BEPLATE—Simulation of Electrochemical Plating

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SUMMARY

BEPLATE is a FORTRAN code that uses the boundary element method to simulate the electrochemical plating of material on parts, primarily rotating axisymmetric parts. A boundary element technique (Appendix A) is used to solve for the local current density and thus the plating rate on the part, which is used to calculate the growth in the plated layer over a user-specified time step. The surface is moved to reflect this growth, and the new surface is used to generate the local current density. This cycle is repeated until the final time specified by the analyst, producing the final plated thickness.

BEPLATE includes models for the polarization effects at both the part (cathode) and anode and allows the use of symmetry planes and nonconducting shields. For electroplating simulations, the part shape is normally assumed to be axisymmetric with a centerline along the z-axis. More general part shapes can be analyzed by BEPLATE if the surface growth simulation is not needed. In either case, the shield, anode, and tank geometries are not restricted to specific shapes.

This report includes the information required to run BEPLATE, specifically, a brief description of the BEPLATE system including hardware and software requirements, a description of the complete simulation process, discussion of rules for generating models, and additional reference material.

This system of codes consists of model generators (PIGS¹ or PATRAN²), input processor (BEPIN³), the simulation code (BEPLATE) and postprocessing codes (PATRAN or CONPLOT⁴).

1. INTRODUCTION

The simulation of electrochemical plating can provide the electroplater with a cost-effective design tool for determining appropriate plating configurations and parameters. Because the cost of plating simulation is much less than that of a plating experiment, significant reductions in the cost of producing a part to a specific tolerance can be achieved in the design of plating cells and shields by using the BEPLATE code. Considerable optimization of plating-cell designs can be achieved with numeric simulation before performing any plating runs.

The BEPLATE system of codes was developed to simulate electrochemical plating, especially the growth of the plated layers on rotating axisymmetric parts. This system consists of two commercial codes, the PAFEC¹ Interactive Graphics Suite (PIGS) code and PATRAN², and two locally developed codes, BEPIN³ and BEPLATE. PIGS and BEPIN are used for model development. BEPLATE performs the simulations, while PATRAN is used to display the model and results (called postprocessing). The locally developed CONPLOT⁴ code can also be used for postprocessing. The analyst is encouraged to become familiar with these codes in order to become adept at producing effective models. Reference 3, which describes BEPIN in detail, will be helpful in developing effective BEPLATE simulations. The manuals for PIGS and PATRAN (or CONPLOT) will be needed and can be obtained from the vendors.

This report, which is intended to function as a general manual for users of BEPLATE, starts with a description of the electrochemical plating processes that can be simulated by BEPLATE (Sect. 2). Section 3 contains a brief description of each component of the system including software and hardware requirements. Section 4 describes the general process of performing a simulation. This process requires adherence to the rules for model generation described in Sect. 5.1. A set of the standard models is included in Sect. 5.2 to help the analyst develop new models or modify old ones. Discussion of the geometry-modification techniques (Sect. 6) and the polarization models (Sect. 7) should help the analyst to develop an effective model. Section 8 contains a detailed step-by-step description of a typical simulation and the resulting datasets. Section 9 discusses various characteristics of the numerical technique of which the analyst should be aware.

The numerical methods used by BEPLATE are summarized in Appendix A (from refs. 5-9). The verification, benchmarking, and validation documentation is contained in Appendix B, and the complete description of the input dataset for BEPLATE is contained in Appendix C.

The generation of a model for BEPLATE is most efficiently performed using the PIGS code to produce the basic geometry of the plating cell, cathode, anode, and shields. (A schematic outline of the complete process is included in Fig. 1.1.) PIGS is an interactive model-generating tool for the PAFEC finite element analysis code. Section 4.1 contains a brief description on how to get started using PIGS. PIGS allows the analyst to easily generate a model using planar triangular elements on the surfaces of all components in the plating cell. The graphics features of PIGS allow the analyst to check the model visually. The analyst runs PIGS, keeping in mind the guidelines for model geometry and other parameters explained in Sects. 5 through 7.

The file geometry produced by PIGS is used as input for the BEPIN code. The analyst chooses the various options or operations in BEPIN using full-

screen, menu-type commands. BEPIN produces a BEPLATE input file, BEPIN.OUT. A PATRAN neutral file, BEPNEUT.DAT, is also produced and can be used with the PATRAN system or the CONPLOT code to check the modified geometry visually. Since BEPIN can modify the geometry, the analyst should make use of this additional check before running BEPLATE. If the model is correct, the BEPLATE input file is transferred to the CRAY X-MP and a simulation is performed.

After the desired simulation has been performed, the BEPLATE-produced model file, BEPLNEU, and results file, BEPLRES, can be transferred back to the VAX to display the results using PATRAN.

Fig. 1.1. Schematic of the BEPIN/BEPLATE process.

2. ELECTROCHEMICAL PLATING/FORMING

Electrodeposition is a process with a long history, much of which is as an art rather than a science. It has been used for aesthetic and decorative purposes as well as for practical engineering objectives.

Decorative use normally entails thin layers ($0.1\text{--}0.3\text{ }\mu\text{m}$) that change the appearance of articles and, at the same time, confer some protection to the object against environmental abuse such as abrasion or corrosion. Common examples are gold plate onto base metal jewelry, chromium onto steel car bumpers, and bronze alloy onto baby shoes. Some archaeological evidence suggests that craftsmen in India used gold plating, powered by a primitive battery, to coat objects around 400 to 500 A.D.

The utilization of electrodeposition for engineering applications is a more recent development, with the plating of materials useful for these purposes being a more technologically difficult task. As with artistic endeavors, protection against deterioration is often the objective. Hard chromium plating of gun barrels and internal-combustion cylinders for abrasion and corrosion resistance are typical applications. Plating is also used extensively as a key step in manufacturing processes such as nickel electroforming of audio recording masters to create record-pressing stampers, copper plating of wiring circuits, gold plating of integrated-circuit lead frames, electroforming of free-standing objects such as the space shuttle rocket engine components,¹⁰ and electrojoining of materials at ambient temperature using electroformed "filler welds."^{11,12} More recent technological applications have generally stemmed either from the desire to produce parts at a lower cost or from designers pushing the requirements for physical and dimensional properties of materials beyond what "traditional" technologies can provide.

In general, the engineering uses of electrodeposition require a greater variety of materials, a higher plating rate, and a thicker and more precise plating layer. Thicknesses on the order of 0.25 cm with tolerances of 0.01 cm are not uncommon. Plating under these conditions is much more difficult, and several problems can arise. In many instances, it is not easy to control the surface morphology and the composition or geometry (thickness profile) of the part, giving rise to such undesirable effects as nodules or trees (dendrites), pinholes, poorly consolidated or embrittled deposits (resulting in poor mechanical properties), "burned" deposits with poor reflectivity, and incorrect thickness profiles. Although some of these symptoms are caused by particulate-control problems, many result from a lack of understanding of, or control over, the basic physical and chemical processes involved.

A major problem in the efficient use of electroplating is, therefore, the limited ability to design a plating cell that will produce a part having the required mechanical and geometrical properties. Currently, this is almost always accomplished by trial and error, relying on the "art" of plating (experience and intuition) to guide the process. An alternative approach to the design problem is to plate a layer thicker than necessary and then machine the part to the correct dimensions. The main drawback of these methods is, of course, that they are time consuming and expensive. This is especially true when a new plating situation is encountered, in which past experience may not be of much assistance. These problems can reduce the attractiveness of applying electroplating technology in new areas.

Computer modeling of electrodeposition can serve two useful purposes. First, simulation can be a replacement for the costly laboratory work required by the cut-and-try design process, thus making it possible to design plating cells quickly and inexpensively. Second, simulation can be used as an experimental device, contributing to the understanding of the plating process itself. Numerical calculations can indicate which of the many factors and parameters are the most crucial in determining the part characteristics and which, therefore, need to be controlled or measured more carefully. By comparison with actual plating runs, simulation can also indicate whether or not all of the important processes have been incorporated in the model. Enhanced understanding of the deposition process would allow a wider variety of materials to be plated at faster rates; together with the ability to economically design the cell, this will make electroplating/electroforming a more versatile and useful technique.

2.1 PHYSICAL PROCESS OF ELECTROPLATING

Electrodeposition is an electrolytic process governed by Faraday's laws of electrolysis.¹³ Electrolysis (literally, breaking down with electricity) occurs whenever charge is transferred between electronic and ionic conductors. The cathodic reaction in plating is the reduction of metal or metalloid ions to the elemental or uncharged state. Following Faraday's laws, the deposition rate is proportional to the current density I (current/area) at the cathode surface, which is directly related to the electrolyte conductivity and the potential gradient near the surface:

$$I = k \frac{\partial V}{\partial \vec{n}}, \quad (2.1)$$

$$\frac{\Delta D}{\Delta t} = \frac{\epsilon M I}{n F \rho}, \quad (2.2)$$

where $(\partial V / \partial \vec{n})$ is the potential gradient with respect to the normal to the surface, D is the position of the surface along the normal, F is Faraday's constant, k and ϵ are the conductivity of the electrolyte and the current efficiency, and M , n , and ρ are the molecular weight, valence, and density, respectively, of the material being plated. Control over the current density distribution on the cathode is therefore a first priority.

The conductivity k is given by

$$k = e \left(\beta_0 + \frac{\beta_1}{T} \right), \quad (2.3)$$

where β_0 and β_1 are parameters that depend upon the electrolyte composition and T is the electrolyte temperature in Kelvin (K). Other than the current efficiency ϵ , the parameters in Eq. (2.2) are easily obtainable. Side reactions can reduce ϵ to a value significantly below 100%, as is the case for chromium

plating from hexavalent chromium electrolyte,¹⁴ and thus a reliable value for ϵ is essential. In fact, the anode dissolution process can also be very inefficient, even essentially zero; in such cases, the anode acts as a current source, though not a material source, and the plated metal must be replenished into the electrolyte. BEPLATE assumes that both the anodic and cathodic current efficiencies are 100%. Although the anode does dissolve, its geometry (which, as will be explained later, is approximate to begin with) is not altered during the simulation; the changes can be minimized and do not have a significant impact on the calculation.

The current density is obtained from the potential field $V(x,y,z)$, which satisfies Laplace's equation

$$\nabla^2 V = 0 \quad (2.4)$$

The boundary of the region consists of insulated surfaces (for which $\partial V / \partial \vec{n} = 0$) and potential surfaces (anode and cathode). The boundary conditions on the electrodes take into account the nonlinear transfer function relating current and potential difference, and thus the entire problem is nonlinear. If $V_0 = V_{0A} - V_{0C}$ denotes the applied voltage difference across the plating system ($V_{0A} \geq V_{0C}$ for the applied anode and cathode potentials), then¹⁵

$$V_0 = (V_{eA} + \bar{\eta}_A) + \Delta V_{ir} - (V_{eC} + \bar{\eta}_C) \quad (2.5)$$

where ΔV_{ir} is the voltage dropped in the electrolyte and $\bar{\eta}_A$ and $\bar{\eta}_C$ are the differences in potential (overvoltage or polarization) from the equilibrium values V_e at the electrode surfaces. [In this discussion, the capital letter subscripts (A or C) refer to the location of the polarization (anode or cathode). The lower-case subscripts (a or c) refer to the type of polarization (activation or concentration).] The boundary conditions on the electrodes for Laplace's equation are,

$$\begin{aligned} V_C &= V_{0C} - \bar{\eta}_C - V_{eC} \ , \\ V_A &= V_{0A} - \bar{\eta}_A - V_{eA} \ . \end{aligned} \quad (2.6)$$

The polarization effectively reduces the amount of voltage that can go into the plating operation ($\bar{\eta}_C$ is negative). Possible voltage drops within the electrodes are neglected in this analysis. The equilibrium potentials at the cathode and anode are assumed identical in BEPLATE. This assumption is appropriate for the electroplating processes examined but is not valid in all cases. The addition

of differing equilibrium potentials at the cathode and anode would require only minor modifications to BEPLATE.

Each overvoltage may be composed of three components due to electron transfer (activation) η_a , mass transfer (concentration) η_c , and resistance effects η_r :

$$\bar{\eta} = \eta_a + \eta_c + \eta_r. \quad (2.7)$$

Resistance polarization is ignored in BEPLATE although it can be easily added. The activation and concentration overpotentials are functions of the current density at the electrode surfaces.¹⁶ The activation overpotential is given by the following Butler-Volmer equation

$$I = I_0 \left(e^{\frac{\alpha_A F}{RT} \eta_a} - e^{-\frac{\alpha_C F}{RT} \eta_a} \right), \quad (2.8)$$

and η_c is determined by

$$\eta_c = \frac{RT}{nF} \ln \left(1 - \frac{I}{I_l} \right), \quad (2.9)$$

where R is the gas constant. The transfer coefficients α_A and α_C are in general different for the anode and cathode; the exchange currents I_0 may be different on the electrodes. All of these parameters are dependent on the specific electrode reactions, electrolyte composition, fluid flow, and the type of material being plated. For example, in the electroplating of rotating axisymmetric parts, the limiting current I_l is a function of the concentration boundary layer at the electrode surfaces and is therefore dependent on the fluid flow created by the spinning part. BEPLATE uses approximations for the boundary layer on the cathode, but the fluid motion near the anode (which is reasonably far away from the spinning part) is ignored.

The functional form used for I_l is

$$I_l = I_{l0} \frac{\delta_0}{\delta}, \quad (2.10)$$

where δ is the thickness of the concentration boundary layer near the electrode through which mass transport perpendicular to the part surface occurs only by diffusion. The outer boundary of this layer is determined by the point at which the electroactive ion concentration is equal to the bulk concentration. This is a thinner layer than the hydrodynamic or momentum boundary layer. The limiting current I_{l0} at the reference boundary layer thickness δ_0 is an experimentally determined quantity. The details of the

concentration polarization models are discussed in Sect. 7. Section 7 also discusses the use of the activation polarization techniques in BEPLATE.

3. DESCRIPTION OF BEPLATE SIMULATION SYSTEM

3.1 SOFTWARE

The BEPLATE system consists of a preprocessor code (PIGS is normally used), a user interface (BEPIN) the numerical simulation code (BEPLATE), and a postprocessor code (PATRAN or CONPLOT). The features and operation of each of these codes are described in the following.

3.1.1 PIGS Code

The generation of a model for BEPLATE is most efficiently performed using the PIGS code to produce the basic geometry of the plating cell, cathode, anode, and shields. (A schematic outline of the complete process is included in Fig. 1.1.) PIGS is an interactive model-generating tool (also called a preprocessor) for the PAFEC finite element stress and heat transfer analysis code. PIGS allows the analyst to easily generate a model using planar triangular elements on the surfaces of all components in the plating cell. BEPLATE uses the boundary element method (BEM) with three-sided linear elements; thus, only the surfaces need to be discretized in triangular elements. The graphics features of PIGS allow the analyst to check the model visually. Sections 4.1 and 8.1 contain brief descriptions on how to get started using PIGS. Reference 1, the user manual for PIGS, more fully explains this interactive graphics-based system. The analyst runs PIGS, keeping in mind the requirements of the BEPLATE code explained in this section and the guidelines for model geometry and other parameters explained in Sects. 5 through 7.

PIGS is the preferred model-generating tool because the discretizations on a curved surface that it produces can be regular (all elements of the same size and shape) and structured in rows. The nodes of such a PIGS-generated discretization will lie along $z = \text{constant}$ lines and elements will not straddle these lines. Such a discretization is consistent with the surface growth technique in BEPLATE (see Sect. 5.1). The uniform size of the elements minimizes local computational errors resulting from local inexactness in modeling the curved surface.

Models of complex three-dimensional (nonaxisymmetric) shapes that don't require simulation of plating that incorporates surface growth can be analyzed using BEPLATE and can be generated by other model-generating codes such as PATRAN. Of course, the analyst may wish to build the model input by keying it into a file without the aid of interactive codes. When using methods other than PIGS, the analyst must be sure that all the necessary requirements of model generation are followed and that the dataset is in the correct format.

Although PIGS has a postprocessing capability, the features and greater power of PATRAN are generally preferred for results display. Therefore, the output neutral and results files of BEPIN and BEPLATE are in PATRAN format.

3.1.2 BEPIN Code

BEPIN is an interactive code that (1) accepts an existing geometry file and (2) uses full-screen menu-type commands to facilitate the generation of an input dataset for BEPLATE. BEPIN uses the VAX/VMS Forms Management System (FMS)¹⁷ to display the screens, make the input easy, and provide screen- and topic-specific help systems. A general help system is provided within the BEPIN code that is very similar in format and function to the VAX/VMS help system.

BEPIN does not perform any analysis; it only prepares a dataset for input into BEPLATE. The model can be slightly modified by the surface-improving techniques. BEPIN allows the analyst to specify the polarization options desired for the analysis. Several dataset modifications can be performed in BEPIN and the correctness of the model can be partially checked using the BEPIN utilities. BEPIN can be used to generate a BEPLATE input dataset from a PIGS output dataset or it can also modify an existing BEPLATE input dataset.

BEPIN will also produce a neutral file that is in the PATRAN format to easily take advantage of the features and greater power of PATRAN to visually check the model.

3.1.3 BEPLATE Code

BEPLATE is a boundary-element code that simulates the electrochemical plating of parts, primarily rotating axisymmetric parts. The boundary-element method (BEM) is used to solve for the local current density and thus the plating rate on the part, which is used to calculate the growth in the plated layer over a user-specified time step. The surface is moved to reflect this growth, and the new surface is used to generate the local current density. This cycle is repeated until the final time specified by the analyst, producing the final plated thickness. This process is called a simulation rather than an analysis because the surface grows in response to the local plating rate and the movement can modify the local plating and thus continued growth.

BEPLATE includes models for the polarization effects at both the part (cathode) and anode and allows the use of symmetry planes and nonconducting shields. The part shape is normally assumed to be axisymmetric with a centerline along the z -axis. The shield, anode, and tank-wall geometries are not as restricted. The model will usually be a symmetric segment of the cell geometry.

BEPLATE requires that the user describe the surfaces of the model by completely covering them with triangular elements in a manner similar to tiling a floor. This process is called discretizing or producing a discretization and is usually performed with a code such as PIGS. (A sketch of a typical electroplating cell is shown in Fig. 3.1 and a BEPLATE discretization for a 45° symmetric segment model is shown in Fig. 3.2.) The discretization of some surfaces can be omitted if they are insulated, planar surfaces that lie on the vertical symmetry planes or the top surface of the electrolyte. As shown in Fig. 3.2, the $z = 0$ plane, the top of the electrolyte, is not discretized. Neither are the symmetry planes, $y = 0$ and $x = y$, discretized. Accounting for these surfaces is more accurately accomplished using special properties of the numerical technique in BEPLATE, and thus, no specific discretization for these areas is required.

Fig. 3.1. Typical configuration of an electroplating cell.

Fig. 3.2. Typical discretization of an electroplating cell—45° model.

In PIGS, the analyst specifies the property number of the elements that define a component of the plating cell as the elements are generated. The property numbers are 1 for cathode, 2 for anode, 3 for tank walls, and 4 for

interposed, thin, nonconducting shields. The rules in Sect. 4 are important to remember to generate effective models using BEPIN/BEPLATE.

The boundary element technique used in BEPLATE is a method of modeling a continuous process with a finite number of nodes. As with any such model, the accuracy of the results depends on the spacing between the nodes. In general, the smallest spacing should be in the region where the most accuracy is desired. Curved surfaces or surfaces with large changes in the local potential require smaller element sizes to produce accurate results. To be sure that the results are not grid-dependent, the analyst should experiment with different node spacings or element sizes.

3.1.4 PATRAN Code

PATRAN is a commercial preprocessing and postprocessing code that is available on the Scientific and Technical Computing (STC) VAX machines. PATRAN enables the analyst to produce graphic displays of the model geometry and the results of the BEPLATE simulation. Using the three-dimensional graphic capability of PATRAN, the analyst can achieve much greater understanding of the results and quickly spot potential errors. PATRAN can be used to produce a color fringe plot that is a perspective depiction of the model in any orientation with the color of each point on the outer surface representing the values of a particular variable at that point. A contour plot on the three-dimensional surfaces and a line plot along specified lines for all variables are also available and very useful. PATRAN can also display the displaced surface of the final plated layer compared with the original surface.

The preprocessing or model-generating capabilities of PATRAN, although powerful, are not suited for electroplating simulations in BEPLATE. PATRAN will generate surface discretizations of linear triangular elements, on a surface that is bounded by only three sides. However, the automatically generated discretizations are irregular and not ordered in the manner required by BEPLATE surface growth techniques. These discretizations could be used in electrochemical analyses that do not require surface growth. The irregular nature of the PATRAN-generated discretization on a curved surface such as a hemispherical surface, can produce errors because of the variation in element size. The region of large elements will produce a more approximate representation of the curved surface than the region of smaller elements. Although the element size varies smoothly, some elements can be much smaller than others on the same surface. Such small elements can produce inaccurate solutions because of the less accurate numerical integration of the singularities. This inaccuracy can be reduced somewhat by increasing the number of integration points at the cost of increasing the computation time. It is possible, although tedious, to produce uniform discretizations from the initial discretization by moving nodes and deleting elements.

3.2 HARDWARE

The hardware requirements of the BEPLATE system include: a suitable terminal or display device, a suitable communications network, appropriate computational capabilities, and the ability to transfer files quickly and easily.

3.2.1 Terminal or Display Device

The BEPLATE system requires two types of terminals or display devices. The PIGS and PATRAN codes require a Tektronix (TEK) 4014 class or 4100 class compatible terminal. PIGS has been executed using the TEK 4014, TEK 4105, and TEK 4107 terminals. PATRAN has been executed using the TEK 4115, TEK 4105, and TEK 4107 terminals. The FMS system used by BEPIN requires a Digital Equipment Corporation (DEC) VT100 or VT200 class compatible terminal. The BEPLATE code does not require a specialized terminal. Thus, a TEK 4100 class compatible terminal capable of operating as a VT100 terminal and several types of VT200 class terminals that have the capability of operating as TEK 4010 terminals are suitable. The most effective terminal has been the TEK 4107, although a TEK 4115 can produce finer detailed fringe plots. No experience has been acquired for newer TEK or DEC terminals.

Several terminal emulating codes on personal computers have the capability of emulating both types of terminals adequately. The BEPLATE system has been used by the following:

- IBM PC/AT, with an EGA graphics monitor, using TGRAF-07 software.
- Apple Macintosh II, with a color monitor, using VersaTerm Pro software.

The most effective technique has been to use the Macintosh II with the VersaTerm Pro software.

The PIGS and PATRAN codes can produce color displays that can be viewed on the color terminals or PCs. Hard copies of these displays can be obtained by attaching a color hard-copy device directly to suitably equipped display terminals. PATRAN can produce *.HRD files, which can be translated into *.DMF files suitable for processing by the DISSPLA software. DISSPLA is available on most of the Oak Ridge Operations-Department of Energy (ORO-DOE) computers and provides a method of transferring these color displays to the FR80 film recording device. The FR80 can produce color slides, microfiche and movie frames. The slides are suitable for examining the results and presentation. Duplicate slides, A-size color prints, or transparencies can be made.

3.2.2 Preprocessing and Postprocessing

Currently, the preprocessing PIGS software is available within ORO-DOE only on the STC VAX/VMS. PIGS is available for other machines, including workstations. Adding PIGS to other computers should require only payment of a multiple license fee to the vendor.

PATRAN is available on the STC VAX (VMS AND ULTRIX) computers. The addition of PATRAN to other computers, including workstations, will require the payment of additional license fees to the vendor.

3.2.3 FMS Software

The FMS software, required by BEPIN, is available on several VAX/VMS computers within ORO-DOE.

3.2.4 Computational Needs

BEPLATE can be executed on many computers, including workstations. The current version requires that the Numerical Algorithms Group (NAG)¹⁸ library routines DO1BAF, F03AFF, F04AJF, and F04AMF and the local CORLIB¹⁹ library routines SPLIN and SEVAL be available. These libraries could be omitted if appropriate replacement routines are added to BEPLATE. BEPLATE has been used extensively on the CRAY X-MP. Most of the experience has been with the CTSS operating system. However, the code has been transferred to the CRAY UNICOS system.

A VAX 8650 or more powerful computer can easily run small BEPLATE problems. When starting a simulation it is sometimes effective to perform an initial simulation entirely on the VAX, using a very crude model and a small number of integration points. Larger problems can be run on such a computer, but the time required to complete the simulation may become excessive. The computational time required for a VAX execution can be as much as 30 times that of the CRAY X-MP. Execution of BEPLATE on the VAX is often less cost effective than on the CRAY X-MP. However, executing BEPLATE on a VAX removes the need to transfer files. This simplification of the simulation process can be important for small problems.

The whole BEPLATE system of codes could be installed on a VAX/VMS workstation. License fees for PIGS, PATRAN, FMS, and NAG library would be required or alternatives developed. Maintaining the system on one computer eliminates file transfers. Although large problems may require long execution times, this option may be cost effective.

BEPLATE has been executed, but not extensively tested, on a Sun 3 workstation. Although BEPLATE should run on other types of workstations, alternatives for PIGS and FMS would have to be developed before the complete system could be transferred to any type of workstation other than VMS. FMS, which is used by BEPIN, is specific to the VAX/VMS environment but could be replaced by another forms-management package. PIGS may be available on some workstations but might be replaced by other preprocessor codes. PATRAN and the NAG library are available on a wide selection of workstations.

A similar BEM code, developed by L. G. Gray, has been extensively used on an IBM 3091, so it might be possible to transfer the BEPLATE code to this machine. It is not known whether PIGS, FMS, and PATRAN are available in this environment.

3.2.5 File Transfer

The current environment for performing an electroplating simulation is to perform the geometry description (using PIGS) and the input preparation (using BEPIN) on a VAX and then transfer this data to the CRAY for the simulation (using BEPLATE). The results of this execution are then transferred back to the VAX for postprocessing (using PATRAN). Unless the simulation is performed on a VAX, transfer of large ASCII files must be performed. To enhance the productivity of the analyst, rapid file transfer between the VAX and the CRAY must be available. ORO-DOE has this capability with the Ethernet connection between the machines and the File Transfer Protocol (FTP) software.

4. STEPS IN PERFORMING A SIMULATION

Efficient generation of a model for BEPLATE requires the use of the PIGS code to produce the basic geometry input for the plating cell, cathode, anode, and shields. PIGS is an interactive model-generating tool for the PAFEC finite element stress and heat transfer analysis code. PIGS allows the analyst to generate a model using linear triangular elements, required by BEPLATE, on the surfaces of all components in the plating cell. The graphic features of PIGS allow the analyst to visually check the model. Section 4.1 includes a brief description of how to begin using PIGS. Reference 1, the user manual for PIGS, more fully explains this interactive graphics based system. Section 8.1 contains a step-by-step description of the use of PIGS to generate a typical model.

The analyst uses PIGS with knowledge of modeling constraints and produces a geometry file. This file is used as input into the BEPIN code. The analyst chooses the various options or operations in BEPIN using full-screen, menu-type commands and produces a BEPLATE input file. BEPIN also produces a PATRAN neutral file that can be used with the PATRAN system on the VAX to check the modified geometry visually. If BEPIN is used to modify the geometry, the analyst should make use of this additional check before running BEPLATE. In addition, it is possible to use the CONPLOT code to check the geometry and display results visually. If corrections are necessary, the BEPLATE input file can be read by BEPIN and changed.

When satisfied with the model, the BEPLATE input file is transferred to the CRAY X-MP and used as input to BEPLATE. The format of this file is contained in Appendix C to assist in minor editing at this stage. However, because the BEPIN code is designed to allow the analyst to input a previously generated file and edit it, editing the file on the CRAY should not be required.

After the desired analysis has been performed, the BEPLATE-produced model and results files can be transferred back to the VAX to display the results using PATRAN. Although PIGS has a postprocessing capability, the features and greater power of PATRAN are generally preferred for results display. Therefore, the output neutral and results files of BEPIN and BEPLATE are in PATRAN format. CONPLOT may also be used on either the CRAY or the VAX to display the results. CONPLOT is less interactive than PATRAN but more powerful than PIGS for postprocessing.

The following sections describe each step in more detail.

4.1 GENERATE THE GEOMETRY FILE USING PIGS

Most of the local experience has been on PIGS version 3.3. The newer, somewhat different, version (4.0) has been used only a little. The use of the newer version will be described in a supplemental document when sufficient experience has been acquired.

On the STC VAX/VMS the following lines should be included in the analyst's login.com file:

```
$ define/nolog    pafec$dev    u2:
$ define/nolog    pafec$check  pafec$dev:[agg.code.pafec.v6pl.check]
$ define/nolog    pigs$lib     pafec$dev:[agg.code.pafec.v6pl.pigs]
$
$ pigs33          == "run pigs$lib:pigs"
```

These statements define the proper symbols for the current system on the STC10 VAX/VMS. Changes in the system or installation of PIGS on other machines will change some of the definitions.

PIGS version 3.3 is executed by typing: *PIGS33*

PIGS will ask what type of terminal; type the appropriate number. When using a Tektronix 4105, 4107, or 4115 terminal, the analyst should type this number. PIGS next asks if a bit pad (digitizer pad) is in use. (At this point when using an IBM PC/AT with the TGRAF-07 emulator, the analyst should type 4105, reset the screen size to 3062 in the graphics parameters menu screen, and set the uppercase lock key on.) The case name is then requested. This and all other input MUST be in UPPERCASE. PIGS will ask for the name of this job.

At this point the analyst should enter the model geometry or read an existing PIGS DI file. The analyst should now enter the LI filename (full name, including extension); PIGS will report the number of nodes and elements in this model and return to the main menu. The analyst should then select the VIEW menu option, which brings up the VIEW menu. This menu allows the display of the model and all of the input features of PIGS.

Normal model input starts with either building construction lines (CONSTR menu option) or defining nodal locations (NOD LOC menu option). These lines or nodes are used to construct the defblocks (DEFBLK menu option) that define the surfaces of the model. The elements are defined on these surfaces by the GENERATE menu option. Always use the linear triangular element (type 39100) and specify the appropriate group and property numbers (group No. = property No.).

After the model has been built as desired, the analyst selects the RETURN menu option to go to the main menu and then the DI SAVE menu option from the main menu to write out a new DI file. Saving the DI file stores all of the current settings, views, and options. This allows the building of new models by slightly altering existing models, or it allows rebuilding of this model with a different element size or configuration. Periodically saving a DI file is recommended to minimize lost effort resulting from mistakes or communication failures. This is the only way that DEFBLOCK, construction line, and node locations can be saved. The last step is usually to select FILE to write out a new PIGS output file for input into BEPIN. You can now exit PIGS and start BEPIN.

The same basic sequence of operations will be used with the newer version of PIGS, but the menus and the method of selecting options will change. Experience gained from using PIGS 3.3 will be useful in using PIGS 4.0 because the concepts of model building are the same.

4.2 DEVELOP PARAMETERS USING BEPIN

BEPIN is an interactive code that uses full-screen, menu-type commands to facilitate the generation of an input dataset for BEPLATE. The BEPIN report fully describes the use of BEPIN, which is described briefly in this section.

The steps described here assume that the default sequence of operations is used. The analyst is first asked to name the input geometry file and to declare the data format and measurement units. BEPIN reports a summary of the geometry information that the analyst can use to verify that the data is correct. The analyst is then asked to name the output file. After these preliminaries are completed, the code asks if the analysis is to be transient and requests the location of the symmetry planes. The code then asks if surface improvement is to be performed. Surface improvement corrects small but computationally significant node-location errors that can result from the geometry-definition process. If so, a sequence of forms is then used to determine the surface-improvement options desired. The analyst can modify the locations of the nodes on any or all components in the model. The data for fluid properties and general parameters are then requested.

The code then prompts for the desired options to be used for the polarization models. The analyst can request that (1) no polarization, (2) concentration polarization, (3) activation polarization, or (4) concentration and activation polarization be performed. The analyst can supply the anode and cathode transfer coefficient and exchange current to define the activation polarization by the Butler-Volmer equation. Concentration polarization can be modeled by an analytical technique for the "standard" part or by a table of user-supplied concentration boundary layer thicknesses for general part shapes. Assistance in estimating such boundary layer thickness profiles can be obtained from the report by Kirkpatrick.²⁰

The analyst is then allowed to select any of four utility functions. These functions are removing unused nodes, removing shield nodes, converting the model from a 90° to a 45° model, and checking the input for incorrect node and element definitions.

The output files are written, and BEPIN is stopped. BEPIN will notify the analyst if an error has occurred and place more detailed information in the BEPLIST.DAT file. A PATRAN NEUTRAL file is also produced.

4.3 TRANSFER GEOMETRY FILE TO THE CRAY

BEPLATE can be used on the VAX, but usually analyses are more cost-effective if performed on the CRAY X-MP. The user must transfer the BEPIN-generated dataset to the CRAY. To transfer a file from the STC VAX to the CRAY, the FTP facility is the most effective method. The help files on the STC VAX contain a description of these processes.

4.4 SIMULATE A PLATING USING BEPLATE

The simulation process usually consists of invoking the executable of the BEPLATE code. If the number of nodes is greater or much less than the default

value of 400, then the main routine should be edited to use an appropriate number for the size of the h and z matrices. These square matrices must be dimensioned to $np + ng + nd + 1$ rows and columns. The number of all nodes, regular and shield, is np . The number of nonedge shield nodes ng is added because each nonedge shield node in the original model represents two nodes on opposite surfaces of the shield. The number of double nodes is nd . BEPLATE replaces each node that lies on the intersection of a specified potential and insulated surface in the original model with a double node pair.

This modified main routine is compiled and linked, and the resulting executable is used for executions with this model. BEPLATE is more cost effective when executed on the CRAY X-MP, but it can be run on a variety of machines. The process for two computers is described. Local users can use the following procedures to obtain the executable, object library, and FORTRAN source code for the default main routine.

4.4.1 CRAY

BEPLATE is run on the CRAY X-MP UNICOS environment using the CFT77 compiler.

4.4.1.1 Executing BEPLATE

The analyst retrieves the BEPLATE executable from CFS and executes the program by typing:

```
cfsi get /beplate/beplate
beplate
```

The input file is assumed to be named beplin. The output files are named beplneu for the neutral file, beplres for the results file, and beplout for the normal output file.

4.4.2.2 Modifying BEPLATE

It may be necessary to modify the BEPLATE main routine source to allow for larger models. The BEPLATE main routine source can be retrieved, compiled, linked with the object library, and executed by typing

```
cfsi get /beplate/beplmain.f      /beplate/beplate.a
cft77 -dp beplmain.f
segldr beplmain beplate.a -l /usr/lib/libnag /usr/lib/libcorlib -o beusr
beusr
```

4.4.2 VAX

BEPLATE has been run on the ORNL STC VAX/VMS computers only.

4.4.2.1 Executing BEPLATE

The analyst executes BEPLATE by typing

```
u2:[agg.be.source]beplate
```

The input file is assumed to be named beplin.dat. The output files are named beplneu.dat for the neutral file, beplres.dat for the results file, and beplout.dat for the normal output file.

4.4.2.2 Modifying BEPLATE

It may be necessary to modify the BEPLATE main routine source to allow for larger models. The BEPLATE main routine source can be retrieved, compiled, linked with the object library, and executed by typing

```
copy u2:[agg.be.source]beplmain.for beplmain.for
for beplmain.for
lin beplmain,u2:[agg.be.source]beplate.obj,sys:naglib,sys:corlib
run beplmain
```

4.5 TRANSFER NEUTRAL AND RESULTS FILE TO VAX

The FTP facility is the best available method of transferring files to the VAX from the UNICOS CRAY.

4.6 EXAMINE RESULTS USING PATRAN

PATRAN is executed on the STC VAX cluster by typing PATRAN. The user then types the appropriate terminal name (usually "4105", "4107" or "4115"). These locally defined symbols stand for the Tektronix 4100 class graphics terminals. Any terminal or PC terminal emulator that is compatible with the TEK 4100 class terminals may be used with PATRAN.

A typical sequence of commands for results display are shown below. The PATRAN system responses are shown in bold, while the analyst responses are in italics. Some of the PATRAN system responses have been shortened by replacing letters with ellipses (...). Comments are placed in the stream of commands and are marked by box borders.

\$ patran

```
=====
P A T R A N
RELEASE 2.3A
COPYRIGHT 1979-1989 PDA ENGINEERING
Customer Number: 00234A
MARTIN MARIETTA ENERGY SYSTEMS / OAK RIDGE, TN
VAX/VMS V5.2 Oct-30-1989 10:01:19
OPERATIONAL LICENSE CONTINUOUS
FROM: Sep-19-1989
TO: Jun-30-1990
=====
```

For information on new features in release 2.3
type HELP,NEW,2.3 from within PATRAN.

ENTER DEVICE MNEMONIC, "?" OR "STOP": 4107

MARTIN MARIETTA ENERGY SYSTEMS / OAKRIDGE, TN
INPUT "GO", "SES", "HELP", PATRAN EXECUTIVE DIRECTIVE OR "STOP".

>go

typing "go" starts the PATRAN system.

GO
PATRAN DATA FILE? 1.NEW 2.OLD 3.LAST 4.STOP

>1

1

PREPARING THE DATA BASE SUB-SYSTEM FOR "NEW" FILE:
"PATRAN.DAT;1"

179 PARTITIONS TO BE INITIALIZED:

MODE? 1.GEOM... 2.ANAL... 3.ANALYZE 4.RES... 5.INTERFACE 6.STOP

>5

The interface option allows the reading of a PATRAN neutral file. This type of file is generated by both BEPIN for geometry checking and BEPLATE for results display.

5
INTERFACE? 1.NEUTRAL 2.NASTRAN 3.IGES 4.END

>1

1

NEUTRAL FILE? 1.CREATE OUTPUT 2.INPUT MODEL 3.END

>2

2

NEUTRAL FILE NAME:BEPLNEU.DAT

DO YOU WISH TO OFFSET ANY NEUTRAL INPUT IDS? (Y/N)

>N

N

THE TITLE CARD FOR FILE "beplneu.dat;1" IS:

b8s45 t8322p2s - finer grid on part solid nonsmooth shield

SHALL WE PROCEED WITH THE READING OF THIS FILE? (Y/N)

>Y

Y

```

05/03/88 14:43:10      2.1
PROCESSING NODE
100
200
PROCESSING ELEMENT
100
200
300
400
NUMBER OF ITEMS READ FROM NEUTRAL FILE:
NUM NODE, ELEM, MATL, PROP, CORD, PRES, FORC, DISP, DEFO,...
292 465 0 0 0 0 0 0 0 0 0
INTERFACE? 1.NEUTRAL 2.NASTRAN 3.IGES 4.END
>E
E
MODE? 1.GEOMETRY 2.ANALYSIS MODEL 3.ANALYZE 4.RESULTS
5.INTERFACE 6.STOP
X
4
RESULTS TYPE? 1.P/FEA MODULE 2.EXTERNAL DATA 3.MODEL
FEATURES 4.END
>2
2
RESULTS? 1.DEFORMED SHAPE 2.ELEMENT 3.DISPLACEMENTS
4.NODAL 5.VECTOR 6.END
X
4
ENTER COLUMN NUMBER FOR NODAL RESULTS
>1

```

The BEPLATE-generated results file is a table of three numbers at each node that are referred to as nodal results in the PATRAN system. The first number is the current density, and the second is the potential for all nodes. The third column of numbers also contains the potential of all normal nodes, but if the node is one of a shield ghost node pair, this column contains the potential of the ghost node. The third column has meaning only for shield nodes and allows the display of the potential of both surfaces of the shield. The surface facing the cathode is represented by the normal nodes and the potential results are contained in column 2. The surface facing the anode is represented by the ghost nodes and contained in column 3.

```

1
DISPLAY? 1.CONTOURS 2.ASSIGNMENT 3.SPECTRUM CONTROL
4.SHOW VALUES 5.X-Y PLOT 6.END
>1
1
INPUT THE RESULTS FILE NAME:
>BEPLRES.DAT
BEPLRES.DAT
DATA WIDTH = 3
FILE TITLE =B8S45 T8322P2S - FINER GRID ON PART SOLID
NONSMOOTH SHIELD
STEP 1 0. S 3600.S/STEP VC=-1.540 TEMP=*****

```

COL.1=NORMAL DERIV, COL.2=POT, COL.3=GHOST POT
 DATA VALUES RANGE FROM -0.125E+00 TO 0.591E-01
 ASSIGNMENT? 1.AUTO 2.MAN... 3.SEMI-AUTO 4.CUR... LEV... 5.END
 >1
 1
 ASSIGNED CONTOUR VALUE CODES FOLLOW:
 A 0.5294E-01 B 0.4065E-01 C 0.2836E-01
 ...
 M -0.9452E-01 N -0.1068E+00 O -0.1191E+00
 PICK PLOT OPTIONS THEN "7.PLOT" TO EXECUTE. (DEFAULT = FRINGE)
 PLOT OPTIONS? 1.CONT...2.FRIN...3.CARP 4...5.HAR 6...7.PLOT 8.END
 >VIEW
 VIEW
 VIEW? 1.AXES ABS 2.A...REL 3.SCREEN ABS 4.SCREEN REL 5....8.END
 >1
 1
 INPUT AXES ABSOLUTE THETA X,Y,Z FOR SCREEN 1
 >90,0,-110
 90,0,-110

The view command allows the analyst to display the model in any orientation. This particular orientation is very effective for the typical electroplating cell.

PLOT OPTIONS? 1.CONT...2.FRIN...3.CARP 4...5.HAR 6...7.PLOT 8.END
 >7

These selections will produce a color fringe plot of the results on the model. Many options are possible in PATRAN and the above sequence is just a sample.

>STOP
 STOP
 RESTART DATA BEING WRITTEN ON 30-OCT-89 10:09:44 TO:
 "PATRAN.DAT;1"

5. BEPLATE-FUNCTIONAL MODELS (GEOMETRIES)

5.1 MODEL-GENERATION RULES

The analyst must keep the following rules in mind when building the discretization using the PIGS code. The steps used in making a model by using PIGS are outlined in Sects. 4.1 and 8.1.

1. The geometry of the part and tank must be in the positive x , y , and z octant and must touch the positive x -axis (Fig. 5.1). (An octant is any of the eight parts into which a space is divided by three coordinate planes.) The z -axis must lie along the axis of rotation of the part and increases from the upper surface of the plating bath to the bottom of the tank, as in Fig. 5.2. Only the symmetric portion of the model must be discretized. Figure 5.2(a) presents a one-eighth segment (or a 45°) model, and Fig. 5.2(b) presents a one-fourth segment (or a 90°) model.

2. All defined surfaces must be completely covered by a set of triangular elements. Other element types (such as quadrilateral) are not acceptable. Insulated surfaces that lie on the symmetry planes do not have to be defined. The tank surfaces must completely enclose the electroplating cell, except for the top surface, which is the electrolyte-air interface. The cathode or anode surface must not have holes or uncovered areas within the symmetric volume segment. Figure 5.3 shows an appropriate model.

Fig. 5.1. Diagram illustrating a block in the positive octant for BEPLATE modeling.

(a)

(b)

Fig. 5.2. Tank model showing positive axes: (a) 45° segment; (b) 90° segment.

Fig. 5.3. Model showing complete coverage of all required surfaces.

3. Each element must have a property number to identify its surface type. The property numbers are:

- 1 Cathode
- 2 Anode
- 3 Tank wall and bottom
- 4 Shield

4. For time-dependent electroplating simulations, the nodes on the cathode must lie in lines that are the intersection of axial planes and the part surface. The nodes must be evenly distributed along these lines. This is required to allow the node-moving technique to function properly. Such a discretization of the cathode surface is shown in Fig. 5.4. Analysis of other discretizations is possible if calculation of surface growth is not required.

The "standard" cathode consists of a short cylinder with a hemispherical cap. This surface is created in two parts during discretization with PIGS. The short cylinder is discretized with triangular elements (type 39100 in PIGS) by specifying the number of elements desired across the width and along the length of the four-sided curved surface that represents the symmetric portion of the cylinder. This will produce a set of evenly spaced elements with

horizontal edges along constant z lines. PIGS can produce uneven node spacing by the specification of a number of element ratios; however, the analyst should use this option with care and in the axial direction only. The integration of the current density (required to simulate the part growth) assumes evenly spaced nodes in the circumferential direction. The symmetric portion of the hemispherical cap is described in PIGS as a curved, three-sided surface. The analyst can produce an acceptable discretization by simply specifying the same number of cell divisions along each of the three sides. Again, unequal-size elements can be specified, but this option should be used with care and only in the axial direction. The analyst must take care to follow the rules in the preceding paragraph when generating a geometry using PATRAN or other methods of discretization.

Fig. 5.4. Example of acceptable discretization on the part or cathode surface. View is along the vertical plane passing through the centroid of the surface.

5. All elements on surfaces with *specified potential* must have vertex nodes that are also vertex nodes in the neighboring elements (Fig. 5.5a). The vertex of one element must not be a midside node on another element (Fig. 5.5b). Every node on such a surface that lies on the edge of an element must be a vertex node of that element. This requirement, called coincident discretization, must also be true at the junction of an insulated surface with a specified-potential surface (Fig. 5.6).

Insulated surfaces or junctions between insulated surfaces do not require coincident discretization, but the analyst must ensure that no gaps are left between elements. (This may be difficult to accomplish on an insulated, curved surface without using coincident discretization, as in Fig. 5.7.) The technique of using overlapping elements to ensure complete coverage has not been tested and should not be used. An example of overlapping elements is shown in Fig. 5.8.

(a) Coincident discretization

(b) Noncoincident discretization

Fig. 5.5. Examples of (a) proper and (b) improper discretizations for regions that require a coincident discretization.

Fig. 5.6. Coincident discretization required at the junction of potential and insulated surfaces.

Fig. 5.7. Diagram showing noncoincident discretization, which will produce gaps on curved surfaces, and coincident discretization, which will not produce gaps.

Fig. 5.8. Overlapping elements, which are not allowed.

6. Large elements next to very small elements can cause inaccuracies (Fig. 5.9). Areas of adjacent elements should not vary by more than a factor of 4.

7. Elements must not be too large (or too small) in the areas of interest. Element size limits are problem-dependent. When the flat, triangular elements are tiled over the curved surface, a faceted surface similar to that of a

gemstone is produced. Large elements on such surfaces produce a few points that act as current attractors. This can produce inaccurate local plating rates in the BEPLATE solution. As the element sizes are reduced, more accurate approximations to the geometry and potential field are possible, and the calculational errors will tend to be reduced. However, reduction below a certain size (which is problem dependent) will produce increasing calculational errors as a result of the inaccuracy of the numerical integrations. These errors can best be detected by observing the trend in results for a series of calculations with successively finer meshes. Even when sufficiently small elements are used, there can still be inaccuracies in the PIGS-generated model. The analyst should consider the use of geometry modification techniques (described in Sect. 6).

8. Warnings will be issued if elements are found with included angles greater than 171° or less than 9° . Such included angles produce elements with bad aspect ratios (length/width) and can reduce the accuracy of the calculations.

Fig. 5.9. Diagram showing adjacent elements with a ratio of areas that is too large. This ratio should not be larger than 4.

9. Surfaces in very close proximity may require small elements in order to define the solution at this location accurately. Very large local errors can affect the solution in other parts of the model. To avoid this problem for anodes that extend to near an insulated surface, the analyst should decrease the element size on the end of the anode and on the tank floor near the anode. In problems in which the cell geometry is not fixed, the analyst should allow a clearance of greater than 10% of the height of the anode, thereby avoiding the requirement for small elements (Fig. 5.10). The size of this clearance may be problem-dependent.

For problems in which the analyst has flexibility in placement of the potential surfaces, it is recommended that anodes or cathodes not contact insulated surfaces, thereby avoiding the need for coincident discretization in this area. Anodes that contact the tank bottom can be and have been used extensively. However, the required coincident discretizations are slightly more difficult to generate, and they limit the geometry modification capabilities of BEPIN and BEPLATE. This limitation will restrict the application of the geometry-modification techniques in performing parametric studies and will hamper optimization procedures.

Fig. 5.10. Model with anode that does not contact the bottom of the tank.

5.2 STANDARD MODELS

These standard models are included to give the analyst patterns to follow. Most of the electroplating simulation experience using BEPLATE has been with plating cells No. 1 and No. 2.

5.2.1 Test Plating Cell No. 1

The basic electroplating cell, shown in Fig. 5.11, is a tank 91.44 cm

(36 in.) square at the bottom and 60.96 cm (24 in.) deep, with the electrolyte level at a depth of 45.72 cm (18 in.). The four anodes are wire-mesh cylinders, radius = 6.35 cm (2.5 in.), filled with lead shot and wrapped in bags to contain the anode sludge. (However, for computational purposes, it is a minor approximation to assume smooth cylindrical anodes.) These electrodes are symmetrically located at the corners of the tank at a minimum spacing of 2.54 cm (1 in.) from the walls and extend the full depth of the fluid. The cathode or mandrel being plated consists of a cylindrical base section, radius = 12.7 cm (5 in.) and height = 5.08 cm (2 in.), capped with a hemisphere of the same radius. This electrode is positioned at the top center of the tank, with the hemisphere toward the bottom and the cylindrical piece just fully submerged in the electrolyte. The part is rotated about the axis of the cylinder. The cathode and anode are potential surfaces, while all other boundary surfaces (tank walls and electrolyte top surface) are insulated or zero current-density regions.

5.2.2 Test Plating Cell No. 2

The second plating-cell configuration is identical to the first, except for the replacement of the cylindrical anodes by those of elliptical cross section. These anodes have a semimajor axis of 5.08 cm (2.0 in.) and a semiminor axis of 1.905 cm (0.75 in.). Four anodes are suspended in the corners of the tank at a minimum spacing of 8.97 cm (3.53 in.) from the corner of the walls and extend to the bottom of the tank. The minor axis of the anode cross section is oriented on one of the two vertical planes that pass through the center and the corners of the tank.

5.2.3 Test Plating Cell No. 3

The third plating-cell configuration is identical to the first, except for the replacement of the flat outer tank walls with a cylinder of radius 64.7 cm (25.5 in.). The anodes are symmetrically located at a minimum spacing of 2.54 cm (1 in.) from the wall.

Fig. 5.11. Top and section view of test plating cell No. 1 configuration.

6. GEOMETRY-MODIFICATION GUIDELINES

BEPLATE and BEPIN have techniques that allow the analyst to modify the geometry of the electroplating cell by moving the locations of specific nodes. This is usually done to ensure that the geometry file passed to BEPLATE is an accurate representation of the intended configuration. These techniques can be used to repeat simulations with slightly different geometries to determine the sensitivity of the results to such geometry changes. The geometry-modification techniques fall into two classes. The first class includes surface-improvement techniques that can be performed by BEPLATE and BEPIN or by BEPIN only. This class is discussed in the BEPIN User's Manual. The second are scaling techniques that can only be performed in BEPLATE for the tank walls and electrolyte depth. Although BEPLATE contains surface-improvement techniques, the capabilities of BEPIN may be easier to use. Only the techniques available in BEPLATE are discussed in the following.

6.1 SURFACE IMPROVEMENTS

PIGS models curved surfaces as bicubic parametric equations that can generate node locations that are slightly in error for curved surfaces that span less than 45° for a single surface definition (or DEFBLOCK, as defined by PIGS). This error increases significantly for curved surfaces that span more than 45° . These nodes are used as vertices of the triangular elements that are tiled over the curved surface. Because of the node location inaccuracies produced by PIGS, inaccurate local plating rates can be predicted by the BEPLATE code. The analyst can design his surface definition to minimize this error by reducing the span of any DEFBLOCK to less than 45° . However, this design approach can result in models having (1) a larger number of nodes or (2) elements that have bad aspect ratios. Instead, the analyst should develop a coincident discretization with the desired element sizes and aspect ratios and then use the surface-improvement technique to move the node locations to the correct surface. These adjustments are usually small but are often significant with regard to the accuracy of the current density on the part. Simply reducing the element size (or increasing the number of elements) on a surface will not reduce the location error but will improve the smoothness of the resulting current density distribution. The current density can still be incorrect because the node locations are still in error for the refined mesh. Relatively coarse mesh (large elements) on the cathode can produce accurate results if the surface improvement technique is used.

When the geometric parameters defining the components of the cell and the nodal locations are inconsistent (e.g., the average radius of the nodes on the cathode is not equal to the input radius), one of three results is possible. If the inconsistencies are small ($<10\%$ variation), the surface-improvement technique should produce a new geometry consistent with the input data. Thus, a limited-range parametric study can be performed by using a single geometry file. If the inconsistencies are large, the surface-improvement technique may move the nodes to unexpected locations or it may stop the execution. The surface-improvement technique should not be used to make large changes in the geometry. Instead, a completely new model should be

generated in PIGS and processed with BEPIN. Elements with bad aspect ratios can be generated by the surface-improvement process, but these should be detected by using the BEPIN and BEPLATE element-checking utilities and by examining the geometry with PATRAN. The analyst should be careful when using these options; BEPLATE does only limited checking for inappropriate models.

Improvement of the cathode surface definition produced by PIGS is usually required to produce accurate current densities. BEPLATE can perform surface improvement on the standard cathode (a short cylinder with a hemispherical cap) only. A more general technique suitable for most axisymmetric cathode shapes is intended for future development. Figure 6.1 presents a comparison of the plated layer thickness between models with and without surface improvement of the cathode only. The results without surface improvement have nonphysical values near the pole. The model with improved cathode surface produces results that are much closer to the experimental values (Appendix B.3).

Fig. 6.1. Comparison of models with improved and unimproved cathode geometry for the shieldless plating case.

Improvement of the anode nodes is not normally required because the small errors produced at the anode have little or no effect on the cathode results. When anodes are close to the cathode, however, more accurate node locations may be required and surface improvement should be used. Anodes that have unusual geometries may also require accurate node locations for accurate results. In addition, if the current density distribution on the anode is of interest, surface improvement may be required.

The "standard" anode geometry is a vertical, right-circular cylinder that extends to or near the bottom of the tank. An anode of a radius or length different from that in the geometry file generated by PIGS can be generated easily with the standard surface-improvement technique by changing the

appropriate BEPLATE input data. All nodal locations will be proportionally scaled to fit on the new anode surface. When the anode contacts the bottom plane, a coincident discretization is required by BEPLATE (see Sect. 5.1). BEPLATE can change the length of an anode that contacts the bottom plane only if the electrolyte depth is changed by the same amount. BEPLATE cannot make a model that has anodes that do not contact the bottom plane from a model with anodes that do contact the bottom plane. This model modification requires the addition of elements to the bottom of the anode and to the bottom plane to complete the surface descriptions, a function that is not implemented. The use of anodes that contact the bottom or walls will limit the analyst in performing parametric studies. Therefore, it is recommended that anodes that contact the tank walls be used only when absolutely necessary or when parametric study or anode configuration optimization is not planned.

The shield is normally quite close to the part and small variations in its surface shape can make large changes in the local current density on the part. Thus, it may be necessary to ensure that the nodes on the shield correctly define a specified part by using the surface-improvement technique. BEPIN can adjust the node locations for the following three types of shield designs: (1) flanged hollow cylinder affixed to a hollow, open hemispherical sector; (2) flanged hollow, open cylinder; and (3) flanged hollow truncated cone. Figure 6.2 presents a comparison of results from models that have unimproved and improved shield geometries. The difference between the results for the unimproved and improved models in Fig. 6.2 is about the same as that of the no shield case in Fig. 6.1. Thus, the use of the shield surface improvement option is also recommended.

Fig. 6.2. Comparison of models with improved and unimproved shield geometry for shielded plating case.

6.2 TANK-GEOMETRY SCALING

The geometry of the tank can be adjusted to change the electrolyte depth and the distance of the walls from the centerline. The tank-geometry-scaling input should be used only when the geometry must be changed. This technique does not move the node locations to a specified surface but only scales the existing locations (x,y,z) to new locations (x',y',z') by the following relationships for the square tank option:

$$x' = \frac{x \ t_h}{x_{max}} , \quad (6.1)$$

$$y' = \frac{y \ t_h}{y_{max}} , \quad (6.2)$$

$$z' = \frac{z \ t_z}{z_{max}} , \quad (6.3)$$

where

- t_h = half of the specified tank width,
- t_z = electrolyte depth,
- x_{max} = maximum x locations of tank nodes,
- y_{max} = maximum y locations of tank nodes,
- z_{max} = maximum z locations of tank nodes.

Nodal locations on cylindrical tanks can be scaled by the following relationships:

$$x' = \frac{x \ t_r}{\sqrt{x^2 + y^2}} , \quad (6.4)$$

$$y' = \frac{y \ t_r}{\sqrt{x^2 + y^2}} , \quad (6.5)$$

$$z' = \frac{z \ t_z}{z_{max}} , \quad (6.6)$$

where

- t_r = specified tank radius.

BEPLATE will change only the z -coordinates of tank nodes for models that have tank walls or bottom contacting the anodes. The equivalent anode node movement (change in anode length) must also be specified for such models or the node movement will not be performed.

These relationships can be applied to a tank of any shape to produce a new geometry. The analyst should be careful when using these options because BEPLATE does only limited checking for inappropriate models.

7. NONLINEAR BOUNDARY CONDITIONS—POLARIZATION

The nonlinear boundary conditions used in BEPLATE model real, measurable, interfacial potential changes in the electrochemical plating/forming system and are specified by the parameters η_a and η_c in Eq. (2.7). The method of determining and using these parameters is discussed in the following.

7.1 ACTIVATION POLARIZATION

The electron transfer polarization, η_a , is given by the Butler-Volmer equation, repeated here from Eq. (2.8).

$$I = I_0 \left(e^{\frac{\alpha_A F}{RT} \eta_a} - e^{-\frac{\alpha_C F}{RT} \eta_a} \right) \quad (7.1)$$

Evaluation of Eq. 7.1 is fairly straightforward, but the nonlinear aspect of this part of the boundary condition (the polarization depends on the local current density and the local current density depends on the polarization) requires that an iterative procedure be used in BEPLATE (Sect. 7.3). The analyst must also consider the modeling assumptions of BEPLATE. These include volume-averaged bath temperature, constant mass diffusivity, and constant (or a specific form of temperature dependency for) electrical conductivity and/or fluid viscosity.

The current version of BEPLATE assumes that the temperature of the fluid is constant and uniform. However, during electroplating the temperature of the bath can vary with time and the local temperature of the fluid at the part surface may not be equal to the volume-averaged bath temperature. BEPLATE requires that the analyst determine an appropriate average temperature of the bath over the plating duration for electrolytic solutions whose parameters vary significantly with temperature. The choice of this time- and volume-average temperature may have significant influence on the results. The choice of a single temperature can be difficult because the electrical conductivity is primarily a function of the volume-averaged temperature while the fluid viscosity is a function of the local temperature at the surface of the part.

It would be possible to add a time-dependent volume-averaged fluid temperature option to the BEPLATE code. This modification should be relatively easy because the BEM requires only that the electrical conductivity be uniform for the whole model for each time-step. The addition of a time-dependent local fluid temperature input parameter for the fluid near the part surface, should also be easy. This modification will affect only the boundary condition evaluation and will allow an effective model for time-dependent fluid temperature and temperature-dependent viscosity.

However, the formulation of the BEM used in BEPLATE requires that the electrical conductivity be constant throughout the volume. Thus, a modeling

technique that would allow the electrical conductivity to vary as a function of the local temperature will require a new formulation.

7.2 CONCENTRATION POLARIZATION—STANDARD PART

For the usual plating configuration described by this simulation system, the cathode is rotated; the limiting current I_l is a function of the concentration boundary layer at the electrode surfaces and is therefore dependent on the fluid flow created by spinning the part. In the BEPLATE code, approximations are used for the the boundary layer on the cathode, and the fluid motion near the anode (which is reasonably far away from the spinning part) is ignored. This concentration polarization is described by Eqs. (2.9) and (2.10), repeated here.

$$\eta_c = \frac{RT}{nF} \ln\left(1 - \frac{|I|}{I_l}\right), \quad (7.2)$$

$$I_l = I_{l0} \frac{\delta_0}{\delta}, \quad (7.3)$$

where δ is the thickness of the concentration boundary layer near the electrode through which mass transport perpendicular to the part surface occurs only by diffusion. The outer boundary of this layer is defined by the point at which the electroactive ion concentration is equal to the bulk concentration.

While I_{l0} and δ_0 of Eq. 7.3 are parameters whose values can be reliably estimated, δ presents a problem. Electrolyte flow past a rotating sphere or cylinder has been investigated theoretically,^{21,22} and formulas for δ have been derived; however, there is no corresponding theory for the sphere/cylinder combination or other more general shapes. As a simple expedient, the code uses an expression for δ for each individual shape on the hemisphere/cylinder part and adjusts the boundary layer thickness on the hemisphere by multiplying a constant times the correlation to achieve a smooth boundary layer at the junction of the two components. The accuracy of this technique is unknown but seems to have been sufficient for the current electroplating experiments (see Appendix B).

Below a spin Reynolds number (Re_d = radius·diameter·angular velocity/kinematic viscosity) of 2,000, the literature indicates that the boundary layer on a hemisphere or a long cylinder is completely laminar (see summary by Kirkpatrick²⁰). Thus, BEPLATE will use a laminar correlation for both the hemisphere and cylinder portion of the part for conditions below Re_d of 2,000. For conditions of Re_d above 2,000 and below 25,000, the flow on a cylinder will be turbulent while the flow on a hemisphere will remain laminar. In this range, the code will use a laminar correlation for the hemisphere and a turbulent correlation for the cylinder.

However, above a Re_d of 550, and until the boundary layer becomes fully turbulent, the literature indicates that spiral vortices may exist on a cylinder or hemisphere. These vortices have been found to produce a spiral pattern of ribs or grooves in the plated layer. This region of undesirable

nonuniformities should be avoided. The exact Re_d for onset of spiral vortices is not known for all geometries and conditions. The $Re_d = 550$ limit is a conservative limit that should avoid the formation of spirals. If additional information were available for the conditions to be simulated that indicated that spiral vortices will not form, an accurate plating simulation may be possible for Re_d greater than 550 using the correlations built into BEPLATE. However, the accuracy of these correlations when spiral vortices do exist is unknown.

Above a Re_d of 25,000 (without a jet or other tripping mechanism to force transition to turbulent conditions), the flow on the hemisphere will start out as laminar at the pole and change to turbulent somewhere along the flow path to the equator. The location of the transition and the effect on the plating is unknown. Therefore, the analyst should avoid this flow regime.

Kirkpatrick proposes that if a turbulent jet impinges on the pole, then the flow on a hemisphere can be made completely turbulent above a Re_d of 25,000. In this regime, the turbulent correlations for the boundary layer thickness may be applicable if the polar jet does not significantly alter the basic flow field. Above a Re_d of 25,000, BEPLATE uses these correlations and is thus assuming that a mechanism to force transition to a turbulent boundary layer (e.g., polar turbulent jet) is always used.

For laminar flow conditions on the cylinder,

$$\delta = 0.25 d Sc^{-1/3} \quad Re_d < 20, \quad (7.4a)$$

$$\delta = 0.392 d Re_d^{-0.15} Sc^{-1/3} \quad 20 < Re_d < 264, \quad (7.4b)$$

$$\delta = 2.76 d Re_d^{-0.5} Sc^{-1/3} \quad 264 < Re_d < 2,000, \quad (7.4c)$$

where

d = diameter of the hemisphere,

Re_d = spin Reynolds number $= r\Omega d/\nu$,

r = radius of the hemisphere,

Ω = rotation speed of the mandrel,

Sc = Schmidt number $= \nu/D$,

D = mass diffusion coefficient,

$$\nu = \text{kinematic viscosity} = e^{\left(\gamma_0 + \frac{\gamma_1}{T}\right)}, \quad (7.5)$$

and on the hemisphere ($Re_d < 25,000$),

$$\delta = F_m \frac{1.14d}{(1-0.207 \theta^2)} Re_d^{-1/2} Sc^{-1/3}, \quad (7.6)$$

where θ on the sphere is the angle from the pole. The factor F_m has been inserted in order that the values for δ agree at the juncture of the cylinder and the hemisphere.

For turbulent-flow conditions on the cylinder ($Re_d > 2,000$),

$$\delta = 12.64 d Re_d^{-0.7} Sc^{-1/3} \quad (7.7)$$

and on the hemisphere ($Re_d > 25,000$ assuming polar jet),

$$\delta = 51.3 d (\cos\theta)^{-0.1} (\sin\theta)^{-0.8} Re_d^{-0.9} Sc^{-1/3} \quad (7.8)$$

In the absence of further data on the onset of spiral vortices, the analyst should avoid simulations in the range of Re_d between 550 and 25,000 that will require concentration polarizations calculations using the correlations in BEPLATE.

As new information is acquired about the effects of spiral vortices and laminar-to-turbulent transitions on polarization, it will be possible to perform simulations in the region from $Re_d = 550$ to 25,000. This is possible because BEPLATE also allows the analyst to input a table of concentration boundary layer thickness as a function of the arc length from the pole or the axial distance from the base of the part ($z = 0$). This option should allow the analyst to describe the concentration boundary layer thickness for any flow regime from analytical correlations, numerical simulations, or experimental data.

Kirkpatrick proposes additional correlations for concentration boundary layer thickness on rotating axisymmetric bodies for laminar [Eq. (7.9a)] and turbulent conditions [Eq. (7.9b)]. These proposed correlations are for more general shapes than the previous literature and could be easily implemented. The analyst could also use these correlations to produce a table of boundary layer thicknesses to be input into BEPLATE.

$$\delta = 1.61 \left(\frac{\Omega}{v} \right)^{-1/2} (\sin\alpha)^{-1/2} Sc^{-1/3} \quad (7.9a)$$

$$\delta = 54.9 \left(\frac{\Omega}{v} \right)^{-0.9} (\sin\alpha)^{-0.1} r^{-0.8} Sc^{-1/3} \quad (7.9b)$$

where

α = local angular slope of the surface,

r = radius from centerline.

Unfortunately, the Reynolds number range that produces laminar or turbulent flow on the generalized rotating axisymmetric part shape is not known. Thus, the laminar correlation can only be used below a Re_d (based on maximum diameter) of 550. This limit is proposed by Kirkpatrick to be low enough to ensure that the flow is completely laminar and free of spiral vortices. If a polar jet is used, then the turbulent correlations can only be used above a Re_d of 180,000. This limit is Kirkpatrick's conservative estimate

for fully turbulent conditions. If a polar jet is not present, then the flow, even at this higher Re_d , will exhibit a transition from laminar near the pole to turbulent near the equator, a condition that is inconsistent with these correlations.

7.3 POLARIZATION ITERATIVE PROCEDURE

The solution of Laplace's equation [together with the nonlinear boundary conditions as shown in Eqs. (2.6), (2.7), (2.8) and (2.9)] necessitates the use of an iterative algorithm. For the first time-step of the simulation, the applied potentials can be used as the initial boundary conditions (equivalently, an initial guess of $\eta = 0$), and the current density is obtained by solving Laplace's equation. New boundary conditions are then obtained from Eqs. (2.6), (2.7), (2.8), and (2.9), and the cycle repeats until the boundary values do not change from one iteration to the next. (It was found necessary to underrelax this iteration to obtain convergence.) For subsequent time-steps, the previous converged values of the polarization should provide a good approximation to the new values and are a natural choice as the initial guess. Therefore, this is the procedure that BEPLATE uses when performing subsequent steps in a time-dependent problem.

8. SAMPLE SIMULATION

This section describes the use of the BEPLATE system for an actual simulation. The model is the same as plating cell No. 1 (Sect. 5.2.1) without the shield. For clarity, the simulation is limited to only the first time step of the simulation without polarization or geometry modification. The first two sets of operations described in Sects. 8.1 and 8.2 constitute the preprocessing step. The last step using PATRAN, described in Sect. 8.4, is usually termed the postprocessing step.

8.1 MODEL-GENERATION USING PIGS

PIGS requires the definition of node points or construction lines. This simple model (Fig. 8.1) will be defined by the definition of node points. The locations of the points used in this model are listed in Table 8.1. The PIGS manual contains a more complete description of the following techniques.

The analyst starts PIGS and picks the VIEW option from the MAIN MENU. The NODE LOC option is then picked, and the analyst is ready to start defining the model. Node locations can be input using the cursor locations by placing the cursor where the analyst wishes a node to be positioned and hitting the space bar. A more accurate method is to type "P" or select the PROMPT mode. In the PROMPT mode, PIGS prompts for the required input with typed lines in the bottom text portion of the screen. The analyst may then type the data for a small set of points that define the geometry (see Table 8.1).

These nodes are used to define surfaces (defblocks) in the DEFBLK menu pick. Each defblock is defined by three or four node locations or construction lines. The order in which the nodes are used to define the defblocks determines the order in which the nodes and elements will be numbered in the model file. Type 1 defblocks are used for four-sided regions, and type 2 defblocks are used for three-sided regions. All discretizations for BEPLATE are two-dimensional or 2D in the PIGS menu. This option will allow the generation of a set of nodes and 2D elements on the surface. The nodes and elements are then generated on each defblock by picking the GENERATE option and specifying the color (for display purposes in PIGS), the group and property numbers, and the number of divisions along each border of the defblock. The group and property numbers should be equal and indicate the type of surface that the element is modeling. These numbers are: 1 for cathode, 2 for anode, 3 for insulated surfaces such as the tank walls, and 4 for nonconducting shield surfaces. After the elements have been generated for each surface, select RETURN to return to the MAIN MENU. Both the DI file (SAVE DI option) and the geometry file (FILE option) should be saved. The geometry file can then be used in the BEPIN code.

Fig. 8.1. Model for sample simulation. Numbers in circles are node numbers.

8.2 INPUT-FILE-GENERATION USING BEPIN

This process is described in more detail in the tutorial section of the BEPIN User's Manual. For this exercise, BEPIN is used only to translate the geometry file into a format that BEPLATE can accept. To do this simply type "run u2:[agg.bc.bepin]BEPIN" and answer the question about the location of the input file. Proceed to the output file screen by typing "RETURN" and answer questions about output location and title. Then select the MAIN MENU by pressing the PF4 key on a VT100 keyboard and select option 11 to generate an output file. BEPIN may be exited now.

Table 8.1 Node locations for sample model

Node	Location		
	x	y	z
1	0.0	0.0	0.0
2	0.0	0.0	7.0
3	0.0	0.0	18.0
4	18.0	0.0	18.0
5	5.0	0.0	0.0
6	3.5355	3.5355	0.0
7	5.0	0.0	2.0
8	3.5355	3.5355	2.0
9	18.0	0.0	0.0
10	12.732	12.732	0.0
11	16.2	16.2	0.0
12	18.0	18.0	0.0
13	12.732	12.732	18.0
14	16.2	16.2	18.0
15	18.0	18.0	18.0

8.3 BEPLATE EXECUTION

The BEPIN output file is then transferred to the CRAY and BEPLATE is run by retrieving BEPLATE from CFS (Sect. 4.4.1.1) and typing "beplate". After execution is complete, the neutral and results files must be transferred back to the VAX for postprocessing (Sect. 4.5). The results can then be processed using PATRAN and hard copies of the result plots can then be made (Sect. 4.6).

8.4 PATRAN POSTPROCESSING

The procedure for looking at results with PATRAN is discussed in Sect. 4.6. Figures 8.2 and 8.3 contain the typical contour plots of the results that would be produced for the first time-step of the sample simulation. PATRAN can produce more effective visuals called color fringe plots. These are much easier to interpret and are valuable for presentations but are difficult to reproduce in this type of document.

Fig. 8.2. Normal derivative on part surface.

Fig. 8.3. Potential values on tank walls

9. USER CONCERNS IN PERFORMING A BEPLATE SIMULATION

This section contains a few suggestions based on the experience with the BEPLATE system.

9.1 NUMERICAL INTEGRATION ACCURACY

BEPLATE allows the user to control the accuracy of the numerical integration by modifying the number of integration points used for all elements. Two parameters, NPT and NPOINT, specify the number of integration points that BEPLATE will use for each element for shield and nonshield elements respectively. Because of the hypersingular terms in the shield equation, more accurate solutions are obtained by specifying more integration points for shield elements than for nonshield elements.

Appendix B.1 describes one of the integration accuracy studies that have been performed. Current experience indicates that NPOINT of less than 4 is usually not accurate enough for electroplating simulations. Until more experience is gained, the recommended procedure is to start with a model that is discretized by a few large elements and a small value for NPOINT (e.g., 4). Either increasing the number of elements, reducing the size of the elements, or increasing the value of NPOINT should improve the accuracy of the results. The refinement process is repeated until the analyst determines that the accuracy of the results is sufficient. Experience has also shown that NPOINT (and NPT) of 12 is more than sufficient for most electroplating simulations.

BEPLATE calculates the total current transferred at the anode and cathode. In a simulation without numerical error, these values should be identical. The difference between these values is called the net current error and is an indication of the average error in the calculations. The correlation of the net current error with the absolute error is justified by data for the concentric sphere verification case in Appendix B. Most electroplating simulations do not have an analytical calculation with which to compare the results to determine the accuracy of the solution. The analyst should use the total current and the relative net current error to estimate the accuracy of the simulation.

If the code fails in the function evaluation routine (CALHZL), it is probably because the selection of the specific integration point value produced an arithmetic failure. Selecting the next higher or lower valid NPOINT will often produce a successful simulation. NPOINT and NPT can take the values 1 through 24.

9.2 DISCRETIZATION ACCURACY

The accuracy of the BEPLATE simulations is limited by the numerical and the discretization accuracy. The discretization error is controlled by the size of the elements, how closely the elements approximate the actual curved

surface, and the relative size of neighboring elements. Appendix B.1 discusses a discretization study for the concentric sphere verification case.

Electroplating simulation experience indicates that, for specified-potential, hemispherical surfaces, the analyst should not use less than five element edges along the circumferential span of 45° or along the arc from the equator to the pole. On cylindrical surfaces, the analyst should use no less than five element edges along the circumferential span of 45°. Axial discretization should be determined from the axial current density gradient on the surface and from the size of the elements of adjacent surfaces. The specification of the grid size by element edges is consistent with the method used by the PIGS and PATRAN model-generation tools. These codes require that the analyst specify a number of segments into which the boundary will be discretized. The elements are then generated to match this discretization. When discretizing a specified-potential surface (an anode or cathode), the analyst should always remember the requirement for coincident mesh (Sect. 5.1).

On anode surfaces, discretizations with as low as three element edges along a 90° span have produced adequate solutions. Such crude models of the anodes seem to produce adequate estimates of the total current and the effect of gross anode geometry changes. If a more accurate current density distribution on the anode is required, then the anode discretizations should comply with the requirements stated for the cathode surfaces.

Discretization error can be accurately determined only by performing a discretization study. The comparison of simulations produced by models with different discretizations is the only general method for determining the discretization error. The analyst is strongly encouraged to perform such studies for each type of model. Such studies should be repeated for a model if significant changes are made in the voltage, temperature, conductivity, or polarization parameters. The need for a new discretization study is more critical when the changes may be expected to produce higher current densities or larger current-density gradients.

9.3 COMPUTATIONAL TIME REQUIREMENTS

The computational requirements of BEPLATE depend on the number of nodes, elements, integration points, and time steps. Table 9.1 contains the computational time for a few models. The computational time requirement in seconds for an analysis of a 45° symmetric segment for a single time step on the CRAY X-MP can be estimated by

$$CPU = 1.9 \times 10^{-4} n_p n^2 \quad (9.1)$$

where

- n = number of nodes,
- n_p = number of integration points.

For problems that have shield nodes, Eq. (9.1) can be modified to

$$CPU = 1.9 \times 10^{-4} (n_p n^2 + n_{ps} n_s^2) , \quad (9.2)$$

where

- n = number of nonshield nodes,
- n_s = number of shield nodes,
- n_p = number of integration points for nonshield elements.
- n_{ps} = number of integration points for shield elements.

Additional time steps will require ~70% of the time required for the first time step for either shield or nonshielded cases. The estimates produced by Eqs. (9.1) and (9.2) will be an approximate minimum cpu time for large problems but will overestimate cpu time for small problems.

Table 9.1 Computational times for electroplating models

Model type	number of nodes	NPOINT	CPU time (s)	Results from Eq. (9.1) or (9.2)
sphere	56	10	4.34	6.0
sphere	462	6	250.55	243.3
no shield	81	6	5.09	7.5
no shield	181	6	30.05	37.4
no shield	181	3	22.19	18.7
shield	334	4	90.97	84.8
shield	446	6	222.0	226.8
shield	172	6	25.0	33.7

9.4 TIME-STEP SIZE

The choice of time-step size can influence the accuracy of the electroplating simulation. For electroplatings with limited duration and simple plating-cell design, very large time steps can be taken. Most plating simulations performed have been similar to the experiment described in Appendix B. These experiments have lasted for ~24 hours. Time-step sizes of up to 5 hours produce nearly the same plated layer thickness as smaller time-step sizes. Of course, the level of accuracy required for an analysis would determine the adequacy of a time step size. In general, for electroplating of thick layers on complex parts, smaller time steps will be required.

It is recommended that the ratio of the maximum plated thickness per time step to the final maximum thickness be less than 0.3. It is also recommended that the ratio of the maximum plated thickness per time step to the minimum distance between the part and the other surfaces be less than 0.1. The accuracy of a time-step size is problem-dependent and this recommendation may be overly conservative for some problems. The analyst

should investigate the accuracy of the time step for each specific type of problem.

The data for one problem is shown in Table 9.2 as an example of a problem wherein the above guidelines for time-step size are exceeded without excessive error. The error is estimated from the ratio of the thickness of the final plated layer (at 20 hours) to that of the case with the smallest time step size. $T_{\min}$ is the minimum and $T_{\max}$ is the maximum thickness of a final plated layer. The thicknesses for the 3600 s case are used as the standards ($T_{\min 0}$ and $T_{\max 0}$). The maximum error in using one time step for the 20-hour simulation is $< 1\%$. This accuracy is usually more than adequate. However, this simulation geometry is relatively simple; more complex geometries with wider ranges of current density would be more sensitive to the time-step size.

Table 9.2 Time-step size accuracy

Time-step size (s)	Number of time steps	$\frac{T_{\min}}{T_{\min 0}}$	$\frac{T_{\max}}{T_{\max 0}}$
3600	20	1.00000	1.00000
7200	10	1.00043	1.00040
72000	1	1.00812	1.00765

9.5 CONVERGENCE OF THE POLARIZATION TECHNIQUE

BEPLATE requires that the polarization technique achieve a relative iteration-to-iteration change of 1.0×10^{-6} within 100 iterations. The simulation will be halted if this condition is exceeded. This criterion has been sufficient for most models if the current density is realistic and the models are physically correct. If the polarization technique fails, first examine the polarization parameters and then the model to make sure that they are physically realistic. Correcting these inputs will usually produce a converged solution. The value of the underrelaxation factor used in BEPLATE can also affect the convergence rate. BEPLATE uses 0.2 for the underrelaxation factor, which has been adequate for most simulations performed. Increasing this factor can reduce the number of polarization iterations and slightly reduce the total execution time.

The comparison of BEPLATE simulations to experimental results has been limited to a few geometries and only one electrolytic solution. Adequacy of the convergence criterion for other situations is unknown.

9.6 LIMITS ON SURFACE GROWTH

The part surface should not be allowed to grow too close to other surfaces without reducing the element sizes on both surfaces in the area of proximity. Retaining large elements when surfaces grow close can produce inaccurate

solutions. Current experience is insufficient to give firm guidelines but suggests that the analyst should be aware of this potential source for errors.

9.7 SYSTEMIC EFFECTS OF VARIATIONS IN PARAMETERS

The various parameters discussed in Sect. 2 control the electroplating simulation. The analyst can adjust these parameters in concert to obtain the desired plated layer thickness distribution. Also, experimental plated layer thicknesses could be used to determine the values of a limited number of these parameters when the others are known with sufficient accuracy.

Electroplating experience and examination of the equations in Sect. 2 indicate some general rules that can be used to structure the parameter modification scheme. From examination of the equations in Sect. 2, it can be determined that variations in the current efficiency, atomic weight, valence, and plated material density cannot influence the normal derivative of the potential. Thus, from Eq. (2.2), the plated layer thickness is proportional to these parameters. The relationship between thickness and these parameters is linear, which implies that the effects of variations in each parameter is additive and proportional for all points. The electroplated thickness should be directly proportional to current efficiency, and atomic weight and inversely proportional to plated density and valence. Also, from examination of the other equations, the plated thickness should be a nonlinear function of the temperature, voltage, exchange current, and transfer coefficient. However, for the conditions and electrolyte used in Appendix B.3, the plating thickness responds in a nearly linear manner when the temperature or voltage is adjusted within a limited range.²³

The additive property means that a specific change in plated layer thickness can be achieved by the variation of either one or a combination of several of these parameters. The incremental changes resulting from a variation can be added together to achieve a change. The additive property also implies that the effect of a change in temperature is indistinguishable from that of a change in one or all of the other linear parameters. For example, changing the voltage can produce the same change in the plated layer as changing the temperature. The effect of any variation of one of these linear variables can be predicted by linear interpolation between two specific variations. The additive property may not hold for variations in nonlinear parameters. The property of proportionality means that the ratio of the change in the plated layer thickness to the original thickness at one point on the surface is the same for all other points. Thus, a density variation will change the plated thickness by the same ratio for all points on the surface. These proportional and additive properties have been observed in numerical experiments. However, there is not sufficient physical experimental data to truly confirm the validity of these properties.

Variations in the linear parameters can only change the plated thickness everywhere by a single ratio. The shape of the thickness distribution as a function of axial distance is not modified by such variations. Only the nonlinear parameters can modify the curvature of this distribution. This can be a vital clue when trying to modify the plating parameters to achieve a desired plating thickness distribution. When trying to find a reasonable match with experimental values, often the shape of the plated layer thickness distribution becomes a more important criterion than the absolute values. After the correct shape has been matched, modification of the linear parameters can be used to achieve a match in the values.

Variation in the parameters related to fluid flow can have other, profound effects on the experimental plating results. For example, electrolyte changes that affect the viscosity parameters, together with specific part rotation rate and temperature values, can move the system into and out of the region of vortex cell formation. This can cause dramatic point-to-point differences in plating rate, leading to generation of very nonplanar surfaces. The exact configuration of these surfaces will be a function of properties both of the electroactive ion and of any additives in the electrolyte.

Precision electroplating requires precise determination of as many variables as possible and precise control of the electroplating cell geometry. These conditions are also required for effective use the BEPLATE simulation system.

10. FUTURE WORK

Although the BEPIN/BEPLATE system has been under development for some time, the system described here should only be considered as an initial step in the development of a complete production system. Nevertheless, this version is capable of aiding electroplaters in designing cells and increasing their understanding of the process. Future versions will require further development of both theory and numerical modeling, with substantial experimental effort to verify the results. Experimental efforts are also needed to examine the boundary layers around rotating axisymmetric parts and to study electroplating under more varied conditions.

In this section, the most important new capabilities that should be added to BEPLATE are discussed. These capabilities include improvement of the geometry-modification and concentration polarization techniques to accommodate more general part shapes, allowing plating on the inner surface of a cathode, improvement of the numerical methods (especially the shield technique), and adding an automatic optimization technique. A preliminary investigation of an optimization technique to determine a suitable anode/shield configuration has been carried out and is a very attractive potential feature of BEPLATE.

10.1 FLUIDS INVESTIGATION

Quantitative knowledge of the fluid dynamic effects on electroplating of rotating axisymmetric parts is not complete. Although it is known that fluid dynamic effects can adversely affect the plating, the magnitudes of these effects are unknown in specific situations. Quantitative experiments in different flow regimes should be performed to define the range for which fluid effects are insignificant and to validate the recommendations and correlations proposed by Kirkpatrick (see Sect. 7).

Specifically, Kirkpatrick proposes that the criterion for avoiding the formation of spiral vortices on a rotating axisymmetric body (and, potentially, grooves in the plated layer) is to operate below a Reynolds number of 550 without a polar jet or above 25,000 with a polar jet. The assumptions behind these criteria could be partially validated by repeating the experiment described in Appendix B.3 at Reynolds numbers of 111,262 and 25,000 with the addition of a turbulent jet as specified by Kirkpatrick. An experiment using the higher Re_d without a jet showed evidence of spiral vortices. Adding the jet at this Re_d would confirm that the spiral vortices disappear. (The experiment at $Re_d = 25,000$, alone, might not be sufficient to prove the lack of spirals because their effect on the plated layer might not be measurable at this Re_d .) This experiment should be repeated at $Re_d = 550$ without a jet to verify the lower criteria. These suggested experiments are at best a minimum set and a complete range would, of course, give more confidence in the criteria.

Plating experiments at different rotation speeds may be sufficient to verify the correlations proposed by Kirkpatrick for the general axisymmetric part under turbulent conditions. However, it is likely that additional mass transfer experiments similar to those proposed by Keyes²⁴ will be required.

These experiments would determine the mass transfer from the dissolution of a deposited layer of benzoic acid on the part. The advantage of the latter type of experiment is that complications caused by the electrodynamic transfer of ions are eliminated. Ideally, these experiments would assist in the development of improved expressions for the calculation of the polarization terms.

10.2 PLATING EXPERIMENTS

At a minimum, a series of plating experiments using different electrolytic solutions, cathode shapes, and anode shapes should be performed. A range of cell voltages, cathode-to-anode spacing, and the ratio of cathode to anode surface areas should be investigated. Comparison of these experiments with BEPLATE simulations will instill a higher level of confidence in the BEPLATE technique and may prompt the addition of new capabilities. These experiments should also improve the guidelines for element size, surface clearances, time-step size, and the number of integration points for accurate simulations.

10.3 SURFACE-IMPROVEMENT TECHNIQUES

Although BEPLATE can produce simulations on many general axisymmetric part shapes, the current surface-improvement technique is limited to the "standard" part definition. It is possible to develop a more flexible technique to allow the analyst to describe a general axisymmetric part shape and have the nodal locations adjusted to lie exactly on the surface. This technique would allow more accurate simulations of different part shapes and should be developed to make the BEPLATE system more general.

10.4 INNER-SURFACE PLATING

The capability to plate on the inner surface of the cathode should be developed. Current models are limited by the concentration polarization and node moving techniques to plating on the outer surface only. The confined geometry associated with such inner-radius plating may make subsequent machining difficult or not possible and more precise plating may be required in these situations. The need to improve the precision of plating is a prime motivation for the development of the BEPLATE system, and thus, the addition of inner-surface plating is a natural extension of the code.

10.5 NUMERICAL METHODS

The numerical approximations employed in BEPLATE can be improved on in the following areas: use of higher-order elements to allow more accurate modeling of curved surfaces with fewer elements, improvements in the treatment of the shield equation to include curved elements, and adding

techniques that would allow accurate solution for models having sharp corners on the electrodes. These modifications should produce a more general, accurate, and cost-effective production tool.

10.6 OPTIMIZATION

A limited study of the determination of an optimum shape and location for the anode and/or shield indicated that an automatic optimization technique can be developed. In situations in which the electroplater must produce a very precise plated layer and is free to design the plating cell, automatic optimization will help reduce the number of confirmational experiments needed to arrive at a solution. Development of optimization procedures for the electrolyte properties and polarization parameters should also be possible.

10.7 WORKSTATION ENVIRONMENT

Further development of BEPLATE should take advantage of the emerging "super-workstation" technology. Some of these machines are multiprocessor computers, and BEPLATE should be redesigned to function efficiently in this environment; work in this direction has already been performed²⁵ and indicates that the boundary element technique is ideal for parallel computation. These machines do have three-dimensional graphics capabilities: the entire simulation process—model definition, discretization, solution, and visualization of results—can be carried out on the workstation (with the possibility of the analysis of large models being done on a main-frame computer). Moreover, it may be possible to incorporate the model generation, BEPIN input processing, and BEPLATE into X-WINDOW based menu-driven user interface. This interface could be more portable (less dependent on particular computers) than the current system and should greatly reduce the time needed for an analyst to learn to use the BEPLATE system effectively.

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Appendix A

NUMERICAL METHODS

A.1 BOUNDARY ELEMENT METHOD

To solve Laplace's equation BEPLATE employs the boundary-element method, which will be briefly reviewed here. A more complete discussion is available in refs. 1 and 2. The fundamental solution or Green's function, $G(X, X_0)$, for the three-dimensional Laplace equation is defined by

$$G(X, X_0) = \frac{1}{4\pi \|X - X_0\|}, \quad (\text{A.1})$$

where $\|X - X_0\|$ is the distance between X and X_0 . As this is the potential of a point charge at X_0 , G satisfies Laplace's equation everywhere except X_0 , where

$$\nabla^2 G(X, X_0) = -\frac{1}{2} \delta(X, X_0), \quad (\text{A.2})$$

where the differentiation is with respect to X and $\delta(X, X_0)$ is the Dirac delta function. Using Green's Theorem, it can be shown that Laplace's equation is equivalent to the integral equation

$$\psi(X_0)V(X_0) - \iint_{\partial R} [G(X, X_0)\nabla V(X) - V(X)\nabla G(X, X_0)] \cdot \vec{n} dS = 0, \quad (\text{A.3})$$

where, again, the gradient and the surface integration are with respect to the X variable and X_0 is an arbitrary point on the boundary ∂R . The function $\psi(P)$ denotes the interior solid angle of the surface at P divided by 4π . For example, if the surface is smooth at P , $\psi(P) = 0.5$, whereas if P is the corner of a cube, $\psi(P) = 0.125$. Equation (A.3) provides, for each X_0 , a linear relationship between the values of V and $\partial V / \partial \vec{n}$ on ∂R , and is the starting point for the boundary-element method. Equation (A.3) follows from Eq. (A.2) and $\nabla V = 0$, and thus any function $G(X, X_0)$ satisfying Eq. (A.2) will suffice. BEPLATE uses a "symmetrized" Green's function, designed to take advantage of the symmetric nature of the plating cell; this will be discussed in Sect. A.1.2.

A closed-form solution of the integral equation Eq. (A.3) usually cannot be achieved. An approximate numerical solution can be obtained by

decomposing the boundary surface as a union of M elements, $\partial R = \bigcup_{m=1}^M T_m$, and approximating the functions $V(X)$ and $\nabla V(X) \cdot \vec{n}$ locally on each element T_m . BEPLATE employs planar triangular elements; the k vertices, $\{Y_k\}$, of the

triangles (henceforth called nodes) situated on ∂R ; and linear interpolation over each triangle. (By using "double nodes"³ where necessary, it can be assumed that for each triangle T_m , either V or $\partial V/\partial \vec{n}$ is specified at all three nodes of T_m .) Using this approximation and rewriting Eq. (A.3) for a node X_0 in the form

$$\begin{aligned} \psi(X_0)V(X_0) + \sum_{m=1}^M \iint_{T_m} V(X) \nabla G(X, X_0) \cdot \vec{n} dS \\ = \sum_{m=1}^M \iint_{T_m} G(X, X_0) \nabla V(X) \cdot \vec{n} dS, \end{aligned} \quad (\text{A.4})$$

a linear equation in the K unknown boundary values of V and $\partial V/\partial \vec{n}$ is obtained. By setting $X_0 = Y_k$ in Eq. (A.4) for $1 \leq k \leq K$ (i.e., letting the singularity of the Green's function be each of the nodes), a system of K linear equations is obtained, which, following the form of Eq. (A.4), can be expressed as

$$H\Phi = Z\Phi_n. \quad (\text{A.5})$$

Here, H and Z are K by K matrices and

$$\Phi = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_K \end{pmatrix}, \quad \Phi_n = \begin{pmatrix} \phi_{n_1} \\ \vdots \\ \phi_{n_K} \end{pmatrix}, \quad (\text{A.6})$$

where $\phi_k = V(Y_k)$ and $\phi_{n_k} = \partial V/\partial \vec{n}(Y_k)$. Depending on which values are unknown, the equations can be rearranged in the usual form $AX = B$. (See refs. 2 and 3 for further details.) Although the matrices A and B can be calculated directly without first forming H and Z (and this would, in fact, reduce the computer storage required), for electrochemical applications it is more desirable to calculate H and Z separately and then do the rearrangement. The reasons for this will be discussed in the following. Having put the equations in the form $AX = B$, X can be obtained by an LU factorization algorithm.

A.1.1 Incorporation of Symmetry Planes

There are basically two ways to incorporate the symmetry planes into BEM models. The first and most obvious is to discretize the symmetry planes as if they were insulated surfaces. This was tried initially in the BEPLATE development and proved to be less than satisfactory: the accuracy of the solution was disappointing and nonphysical oscillations were evident. The problem in this case is the corners formed by the intersection of the electrode surface, a specified potential surface, and the insulated planes. Although this problem can now be treated,⁴ including the planes requires more computational work and data-preparation time. Moreover, for the purpose of electroplating simulations, having discretized surfaces adjacent to the (growing) cathode is very inconvenient.

A more efficient manner of incorporating the symmetry planes is to include them directly into the mathematical formulation by means of a specialized Green's function.

A.1.2 Specialized Green's Function

One of the most powerful features of the boundary-element method is the ability to employ a Green's function specially suited to a particular problem. For example, if a $G(X, X_0)$ partially satisfying the prescribed boundary conditions can be found (this is often the case when symmetry is present), any piece of the surface ∂R whose boundary condition is incorporated into G need not be included in the discretization and calculation. This can save labor and computation time and, as an additional benefit, also improve on the accuracy of the results.

For the plating cell of Fig. A.1, it is an easy task to construct an appropriate Green's function. Consider the 45° section model shown in Fig. A.2. In addition to the $x = y$ and $y = 0$ symmetry planes, the $z = 0$ surface is insulated and can be treated as a symmetry plane. Note that a point source at a surface node $X_0 = (x_0, y_0, z_0)$, combined with a source at a point reflected through the $x = 0$ plane, $X_1 = (-x_0, y_0, z_0)$, namely,

$$G(X, X_0) = G_P(X, X_0) + G_P(X, X_1) \quad (\text{A.7})$$

produces a Green's function that satisfies the zero normal derivative boundary condition on the $x = 0$ plane. Reflecting through all three planes ($z = 0$, $x = 0$, $x = y$) generates all possible combinations of signs and interchanges of x and y and hence the sixteen points $X_j = (\pm x_0, \pm y_0, \pm z_0)$ and $X_j = (\pm y_0, \pm x_0, \pm z_0)$; the required Green's function is therefore

$$G(X, X_0) = \sum_{j=0}^{15} G_P(X, X_j) \quad (\text{A.8})$$

Fig. A.1. Typical configuration of an electroplating cell. Symmetrical 45° segment is shown.

Note that, as shown in Fig. A.2, the cathode is "freely floating" (i.e., there are no insulated elements in contact with the cathode) in the discretization utilizing the specialized Green's function. This freedom is exceedingly convenient for plating simulations for the following reason. During the course of a simulation, the cathode node locations are moved to correspond to the growth of the plated layer. Consequently, if the model in Fig. A.2 were to have the symmetry planes discretized, then the insulated surface elements adjacent to the cathode (i.e., having one or two cathode nodes defining the triangle) would also change as the plating progresses. Eventually, as the part grows, these elements would become sufficiently distorted that the computation must be stopped to generate a new mesh. An alternative strategy, namely starting with suitably large elements adjacent to the cathode, adds an additional constraint to the discretization and might be detrimental to the accuracy of the solution for a reasonably thick part. With the specialized Green's function, there are no elements in contact with the cathode and this problem simply disappears.

Fig. A.2. Typical discretization of an electroplating cell-45° model.

A.1.3 Matrix Factorization and Backsolve

It was found that for some of the plating models examined it was necessary to use a matrix factorization technique that incorporated enhanced precision of the inner product. Using techniques without this capability produced nonphysical results or numerical failure in the factorization process. This capability is available in the specific NAG library subroutines used in BEPLATE. Consideration of this should be made if it is necessary to replace the routines F03AFF and F04AJF.

A.1.4 Treatment of Thin Nonconducting Shields

Shielding is often employed in plating as a means of controlling the current density distribution on the cathode. The shield is generally thin, and can be approximated in the mathematical model as a crack. Until recently, the only general-purpose boundary element technique for treating cracks has

been to subdivide the domain into regions without cracks by adding internal surfaces. These surfaces can greatly increase the discretization labor and computational time required to obtain the solution.

A new boundary element technique for thin cavities that does not require subdividing the region has been developed.^{5,6} For the purposes of electroplating, it can be assumed that the boundary condition on the crack surface is specified as zero flux (or zero normal derivative); the unknown quantity on this part of the boundary is therefore the well-behaved potential distribution.

A shield is modeled as a zero thickness volume by having the two surfaces that would normally represent a thin shield occupy the same spatial location. These surfaces will be denoted by S_A and S_B , for side A and side B. This situation is illustrated in Fig. A.3, where, for clarity, the shield is depicted as having two distinct sides. Nevertheless, the node I on S_A and the corresponding node I' on S_B have the same coordinates. The nodes $\{I'\}$ constitute S_B and are referred to as "ghost nodes"; they are not included in the input but are generated by the computer program. Similarly, the surface elements on S_B are understood to be the same as S_A elements with the direction of the normal reversed; integrals over S_B therefore only differ by a sign from the corresponding S_A integrals.

Fig. A.3 Conceptual model of the shield discretization showing node I and its ghost node I' .

At each point of the shield two equations are necessary because there are two unknown potentials, V_I and $V_{I'}$. The first equation is the usual boundary integral equation for the Laplace equation Eq. (A.3). The second equation (referred to as the shield equation) is obtained by differentiating Eq. (A.3) with respect to X_0 in the direction $\vec{N}$, the normal to the shield at X_0 . This yields

$$\psi(X_0) \nabla_{X_0} V(X_0) \cdot \vec{N} + \int_{\partial R} V(X) \nabla_{X_0} \left(\nabla_X \cdot G(X, X_0) \cdot \vec{n} \right) \cdot \vec{N} dS =$$

$$\int_{\partial R} (\nabla_{X_0} G(X, X_0) \cdot \vec{N}) (\nabla_X V(X) \cdot \vec{n}) dS. \quad (\text{A.10})$$

These two equations give enough independent relations to solve the problem.

The singular integrals arising from Eq. (A.10) require special care; in particular, correct evaluation requires that the interpolation of the potential $V(X)$ on the shield surface be differentiable. The algorithm employed in BEPLATE for accomplishing this is described in ref. 7.

A.1.5 Polarization

The current density is obtained from the potential field $V(x, y, z)$, which satisfies Laplace's equation. The boundary conditions on the electrodes take into account the nonlinear transfer function relating current and potential difference, and thus the entire problem is nonlinear. If $V_0 = V_{0A} - V_{0C}$ denotes the applied voltage difference across the plating system ($V_{0A} \geq V_{0C}$ are the applied anode and cathode potentials), then

$$V_0 = (V_{eA} + \bar{\eta}_A) + \Delta V_{ir} - (V_{eC} + \bar{\eta}_C), \quad (\text{A.11})$$

where ΔV_{ir} is the voltage dropped in the electrolyte and $\bar{\eta}_A$ and $\bar{\eta}_C$ are the differences in potential (overvoltage or polarization) from the equilibrium values at the electrode surfaces. [In this discussion, the capital letter subscripts (A or C) designate anode or cathode polarization. The lower case subscripts (a or c) refer to activation or concentration polarization.] The equilibrium potentials V_{eA} and V_{eC} are equal for the system under consideration [and therefore cancel in Eq. (A.11)], although in general they need not be the same. The boundary conditions on the electrodes for Laplace's equation are, therefore,

$$V_C = V_{0C} - \bar{\eta}_C - V_{eC},$$

$$V_A = V_{0A} - \bar{\eta}_A - V_{eA}. \quad (\text{A.12})$$

The polarization effectively reduces the amount of voltage that can go into the plating operation ($\bar{\eta}_C$ is negative). Possible voltage drops within the electrodes are neglected in this analysis.

Each overvoltage may be composed of three components as a result of electron transfer (activation) η_a , mass transfer (concentration) η_c , and resistance effects η_r :

$$\bar{\eta} = \eta_a + \eta_c + \eta_r \quad (\text{A.13})$$

Resistance polarization is not considered in this work. The activation and concentration overpotentials are functions of the current density at the electrode surfaces. The activation overpotential is given by the Butler-Volmer equation

$$I = I_0 \left(e^{\frac{\alpha_A F}{RT} \eta_a} - e^{-\frac{\alpha_C F}{RT} \eta_a} \right), \quad (\text{A.14})$$

and η_c is determined by

$$\eta_c = \frac{RT}{nF} \ln \left(1 - \frac{|I|}{I_l} \right), \quad (\text{A.15})$$

where R is the gas constant. The transfer coefficients α_A and α_C are different for the anode and cathode; the exchange currents I_0 may be different on the electrodes, but are taken as equal for this work. All of these parameters are dependent on the specific electrode reactions, electrolyte composition, fluid flow, and material being plated. For the plating experiment considered herein, the cathode is rotated; the limiting current I_l is a function of the concentration boundary layer at the electrode surfaces and is therefore dependent on the fluid flow created by the spinning part. In the calculations, approximations will be used for the the boundary layer on the cathode, and the fluid motion near the anode (which is reasonably far away from the spinning part) will be ignored.

The functional form of I_l is

$$I_l = I_{l0} \frac{\delta_0}{\delta}, \quad (\text{A.16})$$

where δ is the thickness of the concentration boundary layer near the electrode through which mass transport perpendicular to the part surface occurs only by diffusion. The outer boundary of this layer is determined by the point at which the electroactive ion concentration is equal to the bulk concentration. This is a thinner layer than the hydrodynamic or momentum boundary layer. The limiting current I_{l0} at the reference boundary layer thickness δ_0 is an experimentally determined quantity.

The solution of Laplace's equation [together with the nonlinear (polarization) boundary conditions Eqs. (A.11-A.16)] necessitates the use of an iterative algorithm. For the first time step of the simulation, the applied potentials can be used as the initial boundary conditions (equivalently, an initial guess of $\bar{\eta}_A = \bar{\eta}_C = 0$), and the current density is obtained by solving Laplace's equation. New boundary conditions are then obtained from Eqs. (A.14) and (A.15), and the cycle repeats until the boundary values do not change from one iteration to the next. (It was found that underrelaxing this iteration improved convergence.) For subsequent time steps, the previous converged values of the polarization should provide a good approximation to the new values and are therefore a natural choice as the initial guess.

In this iterative process, Laplace's equation is solved several times with the same geometry, but with different values of the potential on the boundary (the insulated segments remaining insulated). H and Z (and thus also A) are unaffected by such alterations in the boundary conditions; only the right-hand side, B , changes. Furthermore, because the normal derivative always remains zero on the insulated areas, B is determined by H and the new boundary values of the potential. Since Z does not enter into the computation of B , the program computes H and Z separately and then overwrites Z with A , which, in turn, is overwritten by its LU factorization. Having saved H and the LU factors, the iterative process used to obtain the polarization can proceed with little additional work; a new right-hand side B matrix is computed from the previous solution and the matrix H , and then a new solution is determined from the LU factors (the cycle continuing until convergence). Thus, at each step of this polarization loop, obtaining the required solution of Laplace's equation is essentially reduced to an inexpensive forward-and-back substitution.

A.2 NODE MOVEMENT TO SIMULATE PLATED LAYER GROWTH

The rotation of the mandrel about the vertical centerline is intended to produce an axisymmetric surface. The part starts and remains axisymmetric (when the time-dependent option is chosen). Thus, the part surface can be generated by revolving a curve in the $y=0$ plane about the z -axis (Fig. A.4). The rotation speed of the mandrel is on a significantly faster time-scale than the plating action. Thus, the plating on any circumferential ($z = \text{constant}$) line is obtained by integrating the plating along the line. The local normal on the cathode, in the $y=0$ plane, is calculated from the slopes of lines connecting the node with the two nearest nodes (Fig. A.5). The area-weighted average of these slopes is used as the local slope to allow for nonuniform node spacing. The new location for each circumferential line is calculated along this normal, and the new surface is generated by evenly distributing nodes from the $y=0$ plane to the $x=y$ plane. The new node locations are controlled to maintain the nodes on the $y=0$, $z=0$, and $x=y$ planes to assure that the model surfaces join correctly with the planes of symmetry.

This scheme was examined for a uniform-deposition test case, which produced accurate part growth for all the time-step sizes tried. This technique was also compared with one that used an interpolating spline function to determine the normal and proved more reliable and accurate.

Fig. A.4 Node movement is along the local surface normal.

Fig. A.5 Local normal is calculated from line segments between adjacent node lines.

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Appendix B

VERIFICATION, BENCHMARKING, AND VALIDATION

B.1 COMPARISON WITH ANALYTICAL CASES — VERIFICATION

B.1.1 Cube

The boundary-element code was tested on an insulated cube (i.e., two opposing conducting faces having $V = \text{constant}$ specified and the remaining faces insulated), which also has corners and edges formed by the intersection of potential and insulated surfaces. For this problem, the current density results agreed with the analytical solution to at least six decimal places. However, in this situation the geometry is exact, and because the solution is a constant normal derivative, the linear function interpolation is also an excellent approximation.

B.1.2 Sphere

The BEPLATE code was also tested on a concentric sphere case, the symmetric portion of two concentric spheres each having $V = \text{constant}$ specified. The other surfaces, which are symmetry planes, are incorporated into the special Green's function within BEPLATE. The model used for this case was a 45° symmetric portion of the two concentric spheres (radii = 1.0 and 2.0). If the boundary potentials are picked correctly, then this problem is the same as that of a continuous point source (or sink) at the origin of the coordinate system.¹

$$V = \frac{q}{4\pi k r} \quad (B.1a)$$

$$\nabla V = \frac{-q}{4\pi k r^2} \quad (B.1b)$$

where

- V = potential,
- q = strength of point source,
- k = conductivity of region,
- r = radius.

The value of q/k is found by evaluating Eq. (B.1a) at $r = 1.0$ and $V = -1.0$.

$$\frac{q}{k} = 4\pi r V. \quad (B.1c)$$

The boundary condition at $r = 2.0$ is found from Eq. (B.1a) to be $V = -1/2$.

The results of this model are compared with the analytical current density on the two-concentric-sphere case for one discretization (number of nodes = 463) and one integration accuracy (NPOINT = 10) in Table B.1.

Table B.1 Comparison of analytical and numerical normal derivative results

	Inner sphere	Outer sphere
Analytical	1.0	0.25
BEPLATE max.	1.00070	0.2502139
BEPLATE min.	1.00118	0.2500842

This model was used in a discretization (element-size) study and an integration-accuracy study. The discretization-error study results (Fig. B.1) demonstrate that the magnitude of the error can be reduced to a small value by reducing the size of the elements on both surfaces. The monotonic decrease in error as the element size is decreased is typical of the BEM and other numerical techniques.

Fig. B.1 Discretization-error study for concentric spheres case.

The accuracy of the numerical integration is dependent on the number of integration points used in the circumferential integration of the boundary-element equations. The results from the integration accuracy studies of two models (Fig. B.2) show that increasing the number of integration points can

improve the numerical accuracy for a specific discretization only up to a certain level. This is because of the inaccuracy of the linear triangular elements in modeling a curved surface. As the number of integration points is increased, the BEM produces a more accurate solution to the model that is a faceted, gemstone-like approximation of a curved surface. Increasing the number of integration points increases the computational work without increasing the accuracy. It is only by increasing the number of elements (making the elements smaller) that a more accurate geometric approximation to the curved surface can be produced. The two models producing the results shown in Fig. B.2 have relatively coarse and fine discretizations. The finer model contained more, smaller elements and can achieve a lower maximum relative error.

Fig. B.2 Integration-accuracy study for concentric spheres case.

Another measure of the accuracy of a solution is the error in the total current transferred at the anode or cathode. In a simulation without numerical error, these values should be identical. The difference between these values should be an indication of the average error in the calculations. BEPLATE calculates the total current transferred at the anode and cathode by integrating the local current density over each element and summing for all elements on the surface. The net current (the difference of the absolute values of the currents) and the relative net current error (difference divided by the cathode current) are also reported. The correlation of the relative net current error with the maximum relative current density error is shown in Fig. B.3. The relative net current error appears to reach a minimum before the maximum relative error. This is consistent with the definition of the

relative net current error as an integrated error, while the maximum relative current density error is a local maximum.

Most electroplating simulations do not have an analytical calculation to verify the results of even the linear (no polarization or fixed potential) solution. In such cases, the analyst should monitor the total current and the relative net current density error to determine the accuracy of the simulation.

As a verification of the special Green's function technique, this case was analyzed by using both a 45° and 90° model. The results of these two analyses were identical to seven decimal places.

Fig. B.3 Relative net current error as a measure of integration accuracy.

B.1.3 CONTACT HEAT TRANSFER

Heat transfer across material interfaces through dispersed contacts has been an active area of research and, for our purposes, is of great interest because analytical solutions have been developed and widely used with confidence. Two contact-heat-transfer problems are used as verification cases for the BEPLATE code.

B.1.3.1 Circular Contact

A circular contact area in a half-space with specified constant temperature has an exact analytic solution,¹ and therefore serves as an excellent test of the computational method. Denoting the contact temperature by T_0 , the solution is given by

$$T = \frac{2T_0}{\pi} \int_0^{\infty} e^{-\lambda|z|} J_0(\lambda r) \sin(\lambda a) \frac{d\lambda}{\lambda}, \quad (\text{B.2})$$

where a is the radius of the spot and $r = (x^2 + y^2)^{1/2}$. Differentiating Eq. (B.2) with respect to z and setting $z = 0$, the flux on the contact, $0 \leq r < a$, is

$$-k \frac{\partial T}{\partial z} \Big|_{(z=0)} = \frac{2kT_0}{\pi} (a^2 - r^2)^{-1/2}. \quad (\text{B.3})$$

Note that the flux becomes infinite as $r \rightarrow a^-$ and is zero for $r > a$.

If, for the problem depicted in Fig. B.4, the radius (R) and height (L) of the cylinder are sufficiently large compared with the radius of the spot, the solution should mimic the analytic result for the half-space. Exploiting the symmetry, a one-quarter section (Figs. B.5a and B.5b) is used in the calculation. Note that there are no elements on either the $x = 0$ and $y = 0$ planes or on the insulated portion of the $z = 0$ plane. The edge of the contact requires a highly refined mesh (Fig. B.6) because of the discontinuous flux along this curve. However, this level of refinement does not propagate into the remainder of the model because there are no other surfaces adjacent to the contact region. Away from the contact, the functions are not changing dramatically and the discretization can be fairly crude. The ability to isolate the contact, therefore, greatly reduces the number of nodes and elements in the model, thereby reducing the cost of the computation. An additional benefit is that construction of the grid requires much less time.

(a) Isometric view

(b) Cross section

Fig. B.4 Circular contact concentric to a cylinder.

Fig. B.5 Circular contact discretization.

Fig. B.6 Circular contact discretization near the edge showing the nodes (X1 and X2) used to extrapolate values for node X3.

Grid generation

A discretization that concentrates the nodes near the edge of the circular spot was produced using the PIGS code. A preliminary discretization was first constructed in two regions. An outer annulus next to the edge was decomposed into two rows of elements (three rows of nodes). These nodes were arranged in radial rows to facilitate the extrapolation procedure discussed below. The

elements for the inner disk region were uniform in size and somewhat larger than the outer region. To further refine the edge of the disk, the element sizes were then adjusted in a coordinated manner. This adjustment was accomplished by mapping the uniform elements onto the surface of a sphere centered at the origin and then projecting the nodal locations down onto the $z = 0$ plane. The resulting mesh has a smooth (decreasing) transition in element size from the center to the edge, except at the junction of the two regions discussed above.

Extrapolation

The singular behavior of the flux at the contact edge is almost certain to create difficulties for any general-purpose numerical method. In a direct application of the boundary element method, this discontinuity manifests itself in the form of nonphysical oscillations in the computed flux near the edge of the contact. Instead of monotonically increasing radially from the center of the disk, the flux decreases at an interior node closest to the edge. In trying to respond to the singularity, the computed flux at the edge is quite large, and this apparently causes the depressed value at the adjacent interior node.

Although more-sophisticated approximations (i.e., quadratic elements) are likely to improve the results, it is not clear that this would eliminate the problem. It is conjectured that the observed numerical oscillations stem from trying to solve for a nonexistent quantity, namely the flux on the circular arc, and not from an inadequate functional approximation. If this is the case, then using higher-order elements will not alter this state of affairs. Instead of pursuing this course of action (which nevertheless should be investigated), an alternative strategy has been devised.

Based on the idea that one should not try to compute the flux on the contact edge, the linear equations for X_0 an edge node are not computed. These equations are replaced by ones that determine the flux at the edge by extrapolating from interior nodes. The simplest possible procedure is to use two nodes and linearly extrapolate to the boundary curve: let $P_i = (x_i, y_i, z_i)$, $1 \leq i \leq 3$, denote the coordinates of the three points ($i = 3$ the edge point), and u_i , the corresponding flux (see Fig. B.6). The equation for u_3 is determined by stipulating that the distance between (P_3, u_3) and the line formed by (P_1, u_1) and (P_2, u_2) be a minimum. A little algebra yields

$$u_3 = (1 - t^*) u_1 + t^* u_2, \quad (\text{B.4})$$

where t is formed by the inner (dot) products of the vectors

$$t^* = - \frac{(P_1 - P_3) \cdot (P_2 - P_1)}{(P_2 - P_1) \cdot (P_2 - P_1)}. \quad (\text{B.5})$$

Comparison of results

For the calculations, a contact radius of 0.8 cm was selected and two different outer cylinders were employed. The scale of the first cylinder,

height equal to 5.0 cm and radius equal to 3.0 cm, was chosen to correspond to problems considered by Mikic and Carnasciali.² (Figure B.5a shows the discretization for this calculation). As will be seen from the results, the second cylinder, with a height and radius of 15.0 cm, more closely approximates the half-space geometry. The calculations were performed using a 12-point Gaussian quadrature algorithm for the numerical integrations. The contact and base temperatures were $T_0 = 100^\circ\text{C}$ and $T_1 = 0^\circ\text{C}$, respectively.

The radial heat flux distribution on the contact obtained using the two-point extrapolation is shown in Figs. B.7a and B.7b. In Fig. B.7a, the boundary-element results are compared with a finite-volume calculation³ and the analytical approximation.² The computed results agree quite well, and the approximation method is clearly accurate. Figure B.7b displays the results for both cylinders on an expanded vertical scale. The analytic curve for the larger cylinder is obtained from Eq. (B.3); the curve for the smaller cylinder is again the analytic approximation of ref. 2. The boundary-element results agree with the analytic solution and are somewhat better than the finite-volume method near the edge of the contact.

This case serves to verify the BEM for this very demanding problem although the use of a special extrapolation technique was required. This technique is not intended for the normal electroplating problems, because the extreme singularities are not usually a characteristic of these problems. Also because the extrapolation technique was verified in this problem, the use of this technique in appropriate problems would be correct.

Fig. B.7 Circular contact heat flux distribution obtained from BEPLATE and HEATING6 compared with analytical results.

B.1.3.2 Elliptical Contact

When the contact region is modeled by an ellipse with a large eccentricity, the numerical problems at the tip of the major axis become even more acute. Currie^{4,5,6} has investigated this problem quite extensively using a variety of numerical schemes. Following Currie, an ellipse with an eccentricity of 0.998 has been chosen (semimajor axis = 0.154 cm, semiminor axis = 0.009625 cm), and the outer cylinder has been replaced by a rectangular block having a length and height of 2.54 cm and a width of 1.27 cm. Fig. B.8 displays the geometry for this problem. The side walls of this block (the planes $x = 2.54$ and $y = 1.27$) are insulated surfaces, whereas the bottom ($z = 2.54$) and contact surfaces are held at constant temperature ($T_1 = 0^\circ\text{C}$ and $T_0 = 100^\circ\text{C}$, respectively).

Fig. B.8 Elliptical contact geometry.

Grid generation

To accommodate the strongly singular behavior at the tip, $x, y = 0.154, 0.0$, a preliminary PIGS discretization was produced that had a gradual reduction in element size as the tip of the ellipse was approached. To refine this narrow region sufficiently, this discretization was then adjusted in a manner similar to that used for the circular contact. By mapping the original grid onto a surface (obtained by revolving a parabola around the x -axis) and then projecting the nodal coordinates back down to the contact, the degree of refinement achieved can be modified simply by changing the equation of the surface. This is easily accomplished by altering a few program statements; in this way, several different refinements can be tried without having to generate an entirely new grid with the PIGS code. The mapping technique

allows greater flexibility than is available in the PIGS code for smoothly adjusting element size.

The resultant discretization (Fig. B.9) enables the extrapolation technique to be easily applied for most of the edge curve by extrapolating along constant x (vertical) lines. (The major axis of the elliptical spot is along the x axis of the coordinate system.) Near the tip of the ellipse, this is no longer possible, and therefore the extrapolation was performed along nearly constant y lines.

Fig. B.9 Discretization for elliptical contact model.

Using the extrapolation, the computed heat flux on the contact was a smoothly increasing function out to the edge, even at the tip of the ellipse. The calculations also agreed reasonably well with the results reported by Currie;⁵ a comparison of the heat flux values along the axes of the ellipse is shown in Figs. B.10 and B.11.

Fig. B.10 Elliptical contact heat flux distribution along major axis compared with ref. 5.

Fig. B.11 Elliptical contact heat flux distribution along minor axis compared with ref. 5.

B.2 BENCHMARKING

Benchmarking of computer codes involves the comparison of results from two different codes run on comparable models. In this case BEPLATE was benchmarked against the finite element heat transfer analysis code ADINAT.⁷

B.2.1 Electroplating Linear Solution

The linear solution of the Laplace equation for electroplating is identical to the linear solution of the Laplace equation for heat transfer. Thus, it is possible to benchmark the basic Laplace solution in BEPLATE using ADINAT. Thus, only one time step without polarization is used in the following BEPLATE analyses.

B.2.1.1 Plating cell modeled

An actual plating configuration has been used to compare results. The basic electroplating cell (Fig. B.12) is a tank 91.44 cm (36 in.) square at the bottom and 60.96 cm (24 in.) deep, with the electrolyte level at a depth of 45.72 cm (18 in.). The anodes are wire-mesh cylinders filled with lead shot; however, for computational purposes, it is a minor approximation to assume smooth cylindrical electrodes. These four electrodes, radius = 6.35 cm (2.5 in.) are symmetrically located at the corners of the tank, at a minimum spacing of 2.54 cm (1.0 in.) from the walls, and extend the full depth of the fluid. The cathode or mandrel being plated, consists of a cylindrical base section [radius = 12.7 cm (5.0 in.); height = 5.08 cm (2.0 in.)] capped with a hemisphere of the same radius. This electrode is positioned at the top center of the tank, with the hemisphere toward the bottom and the cylindrical piece just submerged in the electrolyte. The cathode and anode are potential surfaces, while all other boundary surfaces (tank walls and electrolyte surface) are zero current density regions. The applied voltage was chosen to be $V_{OC} = -1.54V$ on the cathode and $V_{OA} = 0.0V$ on the anode.

Exploiting the symmetry of the tank, the computational model is the one-eighth section formed by cutting the tank with planes $y = 0$ and $x = y$. The top of the tank is the $z = 0$ plane, the origin is on the centerline of the tank, and the $x = y$ plane cuts through the cylindrical anode. The symmetry planes are mathematically equivalent to insulated surfaces, and the boundary condition therefore sets the current density equal to zero.

The discretization for the boundary element calculation (Fig. B.13a) was constructed with the flexibility of the method taken into account. The triangular elements on the cathode, which is the principal region of interest for a plating simulation, are much smaller than on any other part of the boundary. In general, the element size increases with distance from the cathode. On the large planar insulated regions, the vertices of two adjacent triangles need not coincide, making it an easy matter to alter the element size. The variation in element area over these planes is quite significant, as can be seen in Fig. B.13a. This discretization has 152 nodes and 165 elements.

Fig. B.12 Electroplating tank geometry.

To obtain a reasonable comparison of the solutions for the current density on the cathode, the ADINAT discretization was designed to yield a nodal spacing on all surfaces of the model at least as fine as the boundary element mesh. Unlike the BEPLATE code, ADINAT requires that all adjacent elements have common vertices, making it more difficult to vary the element size in the model. Therefore, the ADINAT mesh, shown in Fig. B.12b, was required to carry the finer nodal spacing of the cathode throughout the model. At the expense of more development time, a more efficient ADINAT mesh with gradually increasing element size could have been constructed.

Fig. B.13 Discretization of tank for linear electroplating analysis.

The ADINAT model employed 2709 nodes and 510 isoparametric elements. To obtain the current densities on the part, hexahedron elements were required. Using wedge-shaped pentahedrons would have been a direct analog of the BEPLATE discretization, but ADINAT is incapable of reporting current densities for this element shape. The ADINAT discretization was constructed using the PATRAN program.

B.2.1.2 Comparison of results

Figures B.14 and B.15 display the normal derivative values across the cathode surface ($z = \text{constant}$) and down the cathode edge ($x = y$). Calculating the normal derivative, obtained directly in the BEM, requires a little more work in the finite-element approach. The computed functional form over a particular element yields a value of the normal derivative at a node; because there is no continuity of the derivatives across elements, adjoining elements can produce different values for the same node. The reported value is the average over all elements sharing this node. Furthermore, with this discretization, ADINAT is incapable of reporting a normal derivative at the pole of the hemisphere. As might be expected, the differences between the two methods for normal derivative are more significant than for the potential solution.

These analyses were run on the CRAY X-MP, the BEPLATE taking 15 s, compared with 68 s for ADINAT.

Fig. B.14 Comparison of the normal derivative distribution along the $z = \text{constant}$ lines on the cathode.

Fig. B.15 Comparison of the normal derivative distribution along the $y = x$ edge of the cathode.

B.2.2 Electroplating Linear Thermal Solution

A highly idealized model of the thermal processes in the same electroplating tank as in Fig. B.12 is considered as an additional verification problem. The heat generated at the electrode surfaces was modeled by a constant heat flux, and it was assumed that the top (electrolyte/air interface) and the bottom of the tank behaved as insulating surfaces. The temperature of the side walls was maintained at the environmental temperature.

The discretization employed for the thermal analysis was essentially the same as that used for the electroplating simulations with fewer nodes and elements. However, some modifications were required because of the different form of the boundary conditions imposed by the heat transfer problem (Fig. B.16). In the thermal model, the boundary conditions switch from specified temperature to specified flux, requiring the use of double nodes, and hence, a consistent discretization in moving from one plane to the other. With this exception, the nodes and elements in the two models correspond. The ADINAT discretization is the same as in the previous analysis (Fig. B.13b).

The calculated temperature profile along the $y = x$ edge of the cathode is displayed in Fig. B.17. Again, these results were compared with finite-element calculation using ADINAT.

Fig. B.16 Discretization of tank for heat transfer analysis.

Fig. B.17 Comparison of temperature along the $y = x$ edge of the cathode.

B.3 COMPARISON WITH EXPERIMENTS—VALIDATION

Only the data from two experiments have been compared with BEPLATE result for a complete electroplating. These experiments were for the standard electroplating cell configuration No. 1, with and without a standard shield.

B.3.1 ROTATING-PART EXPERIMENT

The first experiment was performed on the standard plating cell configuration No. 1 without a shield. The experiment aimed at depositing lead to an average thickness in the range of 0.125 to 0.250 cm; this was considered large enough to adequately test the computer model, yet small enough not to cause too drastic a change in the dimensions of the mandrel and completely invalidate the fluid-flow approximation. The applied voltage ($V_{0C} = -1.54V$, $V_{0A} = 0.0V$) was chosen to cause an average current density in the range of 0.035 to 0.070 A/cm². At 100% current efficiency at both anode and cathode, this corresponds to a plating rate between 0.0119 and 0.0237 cm/h. The total plating time was 1213 min. A lead fluoborate/fluoboric acid/boric acid electrolyte with sodium lignin sulfonate and coumarin additives was used. This is essentially the plating system described by Wiesner.⁸

The mandrel was dimensionally inspected before, and the plate-on-mandrel combination, after the plating run. Four transpolar scans, 45 azimuthal degrees apart, yielded eight values of thickness at each latitude on the hemispherical section and each elevation on the cylindrical section. These

eight values were averaged to yield the experimental thickness against which the calculation was compared.

B.3.1.1 Tank discretization

Exploiting the symmetry of the tank, the computational model is the one-eighth section formed by cutting the tank with the planes $y = 0$ and $x = y$, shown in Fig. B.12. The top of the tank is the $z = 0$ plane, the origin is on the centerline of the tank, and the $x = y$ plane cuts through the cylindrical anode.

The discretization, consisting of 292 nodes and 465 elements, was constructed using PIGS. The cathode surface was smoothed, but no other adjustments to the node locations were performed.

B.3.1.2 Experimental parameters

For the lead-plating system used here, not all of the needed data are known precisely. However, enough information is available to be able to make reasonable estimates for the parameters.^{9,10}

The values used for the parameters of the lead-plating system are summarized in Table B.2.

Table B.2. Parameters for lead-plating system

Symbol	Parameter	Value	Units
ϵ	Current efficiency	1.0	
M	Atomic weight	207.19	gm/mol
n	Valence of ion being plated	2	$\left(\frac{\text{mol electron}}{\text{mol element}}\right)$
F	Faraday's constant	96485	C/equiv
ρ	Density of plated material	11.4	gm/cm ³
T	Temperature	304.9	K
V_{OC}	Applied cathode voltage	-1.54	V
V_{OA}	Applied anode voltage	0.0	V
α_C	Transfer coefficient	0.5	
α_A	Transfer coefficient	0.6	
I_0	Exchange current density	0.0168	A/cm ²
δ_0	Boundary layer thickness	0.002	cm
Ω	Rotation speed	π	rad/s
β_0	Exponential term 0(conductivity)	2.86832	
β_1	Exponential term 1(conductivity)	-1225.86	K
γ_0	Exponential term 0(viscosity)	-10.6296	
γ_1	Exponential term 1(viscosity)	1762.84	K
I_{l0}	Limiting current density (@ $\delta = \delta_0$)	0.5	A/cm ²
R	Gas constant	8.314	J/K mol

B.3.1.3 Comparison of results

The initial solutions (i.e., no plating on the cathode) for the normal derivative before polarization are shown in Fig. B.18. The current density variation is smooth and appears to be physically reasonable. In the absence of data for direct comparison, these qualities are valuable indicators of the correctness of the numerical simulation.

It was possible to measure the experimental total plating thickness distribution, which is plotted in Fig. B.18 together with the results from the computer simulations. The plated layer thickness distribution shows a reasonable agreement, with the exception of the magnitude of the thickness on the cylinder.

There are several factors that may cause significant error. Not all of the parameters were known or measured precisely. In particular, the voltage source in the plating was not the constant $V_{OC} = -1.54V$ assumed in the calculations but fluctuated around this value; experimental modifications needed to record the voltage as a function of time are being implemented. In addition, the temperature was measured near the outside wall of the tank, rather than at the most critical area near the cathode. In this region the current density is a maximum thus producing higher amounts of Ohmic heat (I^2R). Test calculational runs indicated that relatively small changes in temperature could produce noticeable effects on the current density; thus, in subsequent plating runs the temperature will be measured close to the cathode. Also, the approximations of the concentration polarization model (Sect. 7), although possibly of second order, may be the source of additional errors. The comparison in Fig B.19, indicates that the BEPLATE technique can simulate an electroplating with sufficient accuracy to predict electroform growth.

The simulation required 107 s on the CRAY X-MP using six integration points for all elements.

Fig. B.18 Normal derivative distribution on the part surface—no shield case.

Fig. B.19 Plated thickness distribution compared with experiment—no shield case.

B.3.2 Rotating Part with Shield Experiment

The second experiment was performed on the "standard" plating-cell configuration No. 1 with a shield of "standard" design. The experimental conditions and inspection process were similar to the first experiment. The total plating time was 1560 min.

B.3.2.1 Tank discretization

The same plating cell and part mandrel were used in the second experiment with the addition of a shield consisting of a flanged, hollow cylinder affixed to a hollow open hemisphere.

The discretization in Fig. B.20, consisting of 446 nodes (88 were shield nodes) and 605 elements, was constructed using PIGS. The cathode and shield surfaces were smoothed using the standard BEPLATE techniques.

B.3.2.2 Comparison of results

The initial solutions (i.e., no plating on the cathode) for the normal derivative before polarization are shown in Fig. B.21. As in the first experiment, the current density is smooth and appears to be physically reasonable. The plated layer thickness show a reasonable agreement, with the

exception of the sudden rise in experimental thickness at $z \approx 7.0$ (Fig. B.22). This may be an artifact of unknown fluid dynamics effects although limited fluid dynamic analyses showed no such phenomena. It is possible that this is an experimental or measurement error. The existence and cause of the feature can only be determined by the planned repetition of this experiment. As with the first experiment, not all of the parameters are known precisely and these may be the cause of the differences between the experimental data and the calculational results. The placement of the shield close to the rotation part should affect the local fluid flow. The magnitude of the effect is not known and neither is the effect on plating.

The computer time required for the simulation was 176 s on the Cray X-MP. The number of integration points was six for all elements.

Fig. B.20 Discretization of the rotating part with shield model.

Fig. B.21 Normal derivative distribution on the cathode.

Fig. B.22 Comparison of plated layer thickness with experiment—shield case.

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Appendix C

BEPLATE INPUT DESCRIPTION

This appendix briefly describes the input to BEPLATE. Each card is described by listing the input variables, the variable type, and a brief description of each variable. The numeric input consists of a list of floating-point or integer values separated by commas or blanks. Each input variable must be input; default values are usually chosen by the integer "0" (zero).

"I" indicates that the input field will be read as an integer; if a floating-point number is input, it will be truncated. "R" indicates that the number may be either floating point or integer. "C" indicates that the input field will be read as character data. The units of all geometry variables may be all in inches (inch=1) or all in centimeters (inch=0). The "INCH" variable must indicate the appropriate units. If units are specified in the description field for a variable, then the input values must be in the specified units.

Comments may be placed in the data anywhere after the title line. Comment lines must start with an asterisk in the first position.

The following order of the line types must be observed. Line types must be in sequence unless a control variable dictates that a specific line type should be skipped.

First line type—Title of the dataset

1 entry (C)

1. TITLE (C) —Up to 80 characters but only one line allowed

Second line type—Control parameters

13 entries (2I,2R,I,4R,4I)

1. MNODES (I) —Number of nodes in the problem
2. KEL (I) —Number of elements in the problem
3. STIME (R) —Initial time of problem (s)
4. FTIME (R) —Final time of plating simulation (s)
5. NTIME (I) —Number of time steps for plating simulation
6. DELTAT (R) —Time-step size (s)
7. XSYM (R) —Location of the three orthogonal insulated
8. YSYM (R) planes incorporated into the specialized Green's
9. ZSYM (R) function (in. or cm)
10. INCH (I) —Input measurement units: 1 = in.; 0 = cm
11. NPOINT (I) —Number of integration points for nonshield elements
12. NPT (I) —Number of integration points for shield elements
13. NSOLCK (I) —Flag to control solid angle checking: 0 = yes, 1 = no

Third line type—General parameters

3 entries (3R)

1. VCATH (R) —Cathode potential (V)
2. VANOD (R) —Anode potential (V)
3. OMEGA (R) —Rotational speed (rad/s)

Fourth line type—Electrolyte/plate parameters

7 entries (5R,2I)

1. TBATH (R) —Bath temperature ($^{\circ}\text{C}$)
2. PDEN (R) —Density of plated material (g/cm^3)
3. DIFF (R) —Mass diffusivity of ion being plated (cm^2/s)
4. ATWT (R) —Atomic weight of plated material (g/mol)
5. VAL (R) —Valence of metal ion being plated
(mol/mol element)
6. IEK (I) —Electrical conductivity control:
0 = constant conductivity ;
1 = temperature-dependent conductivity
7. IUNU (I) —Viscosity control:
0 = constant viscosity;
1 = temperature-dependent viscosity

Fifth line type—Electrical conductivity

1 entry if IEK = 0 (R)

1. EK (R) —Constant fluid electrical conductivity (A/V)

2 entries if IEK = 1 (2R)

1. BETA0 (R) —First coefficient for temperature-dependent electrical conductivity
2. BETA1 (R) —Second coefficient for temperature-dependent electrical conductivity

Sixth line type—Viscosity

1 entry if IUNU = 0 (R)

1. UNU (R) —Fluid viscosity (cm^2/s)

2 entries if IUNU = 1 (2R)

1. GAMMA0 (R) —First coefficient for temperature-dependent viscosity
2. GAMMA1 (R) —Second coefficient for temperature-dependent viscosity

Seventh line type—Node adjustment control data

4 entries (4I)

1. IADJC (I) —Cathode node adjustment control:
0 = no adjustment
1 = adjust cylinder/hemisphere
or hemisphere cathode
2. IADJA (I) —Anode node adjustment control:
0 = no adjustment
1 = adjust cylinder anode

3. IADJS (I) —Shield node adjustment control:
 0 = no adjustment
 1 = adjust cylinder/hemisphere or hemisphere shield
 2 = adjust cylinder shield
 3 = adjust truncated cone shield
4. IADJT (I) —Tank node adjustment control:
 0 = no adjustment
 1 = adjust square tank model
 2 = adjust cylindrical tank model

Eighth line type—Cathode geometry data

— Read if IADJC = 1 (units are in. or cm)

2 entries (2R)

1. RCYL (R) —Radius of cathode
 2. HCYL (R) —Height of cylindrical portion of cathode

Ninth line type—Anode geometry data

— Read if IADJA = 1 (units are in. or cm)

4 entries (4R)

1. XAC (R) —x-coordinate of the center of anode
 2. YAC (R) —y-coordinate of the center of anode
 3. RA (R) —Radius of anode
 4. ZANO (R) —Length of anode

Tenth line type—Cylinder/hemisphere shield geometry data

— Read if IADJS = 1 (units are in. or cm)

5 entries (5R)

1. RCYLS (R) —Radius of the cylindrical portion of shield
 2. HCYLS (R) —Height of the cylindrical portion of shield
 3. TOPS (R) —Minimum z-coordinate of shield
 4. RFLANG (R) —Flange radius
 5. ANGOPN (R) —Angle of the open section of shield (degrees)

Eleventh line type—Cylinder shield geometry data

— Read if IADJS = 2 (units are in. or cm)

5 entries (5R)

1. RFLNGO (R) —Flange outer radius
 2. RFLNGI (R) —Flange inner radius
 3. ZFLANG (R) —z-coordinate of flange
 4. TOPS (R) —Minimum z-coordinate of shield
 5. ZCYSB (R) —Maximum z-coordinate of shield

Twelfth line type—Truncated cone shield geometry data
 — Read if IADJS = 3 (units are in. or cm)

5 entries (5R)

1. RFLNGO (R) —Flange outer radius
2. RFLNGI (R) —Flange inner radius
3. ZFLANG (R) —z-coordinate of flange
4. ROPEN (R) —Radius of opening
5. ZCONEO (R) —z-coordinate of opening

Thirteenth line type—Tank geometry (units are in. or cm)

3 entries (1,2R)

1. TNKTYP (I) —Type of tank: 0 = square; 1 = cylindrical; 3 = other
2. TSIDE (R) —Tank radius or length of side
3. ZTANK (R) —Maximum z-coordinate of tank

Fourteenth line type—Polarization control

3 entries (2I,R)

1. IBUTVL (I) —Activation polarization control: 0 = no; 1 = yes
2. ICPOLR (I) —Concentration polarization control:
0 = no; 1 = analytical; 2 = tabular
3. ORVAL (R) —Underrelaxation factor for polarization iterations

Fifteenth line type—Butler-Volmer equation parameters

— Read if IBUTVL = 1

4 entries (4R)

1. ALPHA A (R) —Anode transfer coefficient
2. ALPHA C (R) —Cathode transfer coefficient
3. XIO A (R) —Anode exchange current (A/cm^2)
4. XIO C (R) —Cathode exchange current (A/cm^2)

Sixteenth line type—Analytical parameters for boundary layer thickness

— Read if ICPOLR = 1

2 entries (2R)

1. XILIM (R) —Limiting current at DELTA0 (A/cm^2)
2. DELTA0 (R) —Reference concentration boundary layer thickness (cm)

Seventeenth line type—Tabular concentration boundary layer thickness
 — Read if ICPOLR = 2

4 entries (2R,2I)

1. XILIM (R) —Limiting current at DELTA0 (A/cm^2)
2. DELTA0 (R) —Reference concentration boundary layer thickness (cm)
3. IWHERE (I) —Unit number for reading table
4. IZARC (I) —Independent variable flag:
 0 = axial distance from base
 1 = arc length from the pole

If IWHERE is greater than 0, the file TABNAM (line type 18th) will be read for the 19th and 20th line types.

Eighteenth line type—File name for table dataset
 — Read if IWHERE < 0

1 entry (C)

1. TABNAM (C) —File name of table dataset (up to 32 characters)

Nineteenth line type—Table control
 — Read if ICPOLR = 2

1 entry (I)

1. NUMTAB (I) —Number of pairs in the table

Twentieth line type—Table pairs (repeat NUMTAB times)
 — Read if ICPOLR = 2

2 entries (2R)

1. ZTAB (R) —Independent value, axial distance or arc length
2. BLTK (R) —Concentration boundary layer thickness

Twenty-first line type—Node descriptions (repeat MNODES times)

4 entries (I,3R)

1. N (I) —Node number
2. XYZ(N,1) (R) —x location (in. or cm)
3. XYZ(N,2) (R) —y location (in. or cm)
4. XYZ(N,3) (R) —z location (in. or cm)

Twenty-second line type—Element descriptions (repeat KEL times)

5 entries (5I)

1. NE (I) —Element number
2. NPROP(NE) (I) —Property number
3. NODES(NE,1) (I) —Node number of first vertex of element
4. NODES(NE,2) (I) —Node number of second vertex of element
5. NODES(NE,3) (I) —Node number of third vertex of element

Twenty-third line type—Orientation point locations (optional input)

Supply this line type to override the default orientation points; omit to use the defaults. Twelve entries must be supplied; continue on as many lines as required. (units are in. or cm)

12 entries (12R)

1. PT(1,1)	(R)	—x-coordinate of the orientation point for the elements with property number 1.
2. PT(1,2)	(R)	—y-coordinate of the orientation point for the elements with property number 1.
3. PT(1,3)	(R)	—z-coordinate of the orientation point for the elements with property number 1.
4. PT(2,1)	(R)	—x-coordinate of the orientation point for the elements with property number 2.
5. PT(2,2)	(R)	—y-coordinate of the orientation point for the elements with property number 2.
6. PT(2,3)	(R)	—z-coordinate of the orientation point for the elements with property number 2.
7. PT(3,1)	(R)	—x-coordinate of the orientation point for the elements with property number 3.
8. PT(3,2)	(R)	—y-coordinate of the orientation point for the elements with property number 3.
9. PT(3,3)	(R)	—z-coordinate of the orientation point for the elements with property number 3.
10. PT(4,1)	(R)	—x-coordinate of the orientation point for the elements with property number 4.
11. PT(4,2)	(R)	—y-coordinate of the orientation point for the elements with property number 4.
12. PT(4,3)	(R)	—z-coordinate of the orientation point for the elements with property number 4.

END

DATE FILMED

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