22,094

LATTICE STATICS OF INTERSTITIALS IN TUNGSTEN

by

Roy Benedek
Department of Materials Science and Engineering
Cornell University
Ithaca, New York 14850

and

P. S. Ho
IBM Thomas J. Watson Research Center
Yorktown Heights, New York 10598

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

Issued by

The Materials Science Center

Report #2013

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

ABSTRACT

A modified Green's function approach suggested earlier by the authors has been applied to the calculation of lattice distortion fields and energies and volumes of formation for six interstitial configurations in Tungsten. Two interatomic potentials, one fitted to the phonon spectrum and the other, derived by Johnson and Wilson, to elastic constants, were used in numerical calculations. Results for the energy of formation show considerable sensitivity to the form of the potential, as expected from previous work. An expression is derived for the volume of formation which includes a correction to the standard formula involving the defect strength divided by the bulk modulus. This correction term depends explicitly on the volume dependent part of the crystal energy and vanishes for a Cauchy crystal.

1. INTRODUCTION

In a previous paper (Benedek and Ho 1973, hereafter referred to as I) the Green's function approach to the calculation of lattice distortion surrounding point imperfections was adapted to the case of interstitial defects. Such defects introduce a rather large distortion into a crystal lattice and therefore require special treatment. An approach was developed based on treating a selected region (the "core") near the defect formally as a cluster of $n+1$ "interstitials" and n "vacancies". By a judicious choice of the atoms to be included within this core and their initial positions one ensures the validity of the "harmonic approximation" implicit in the Green's function equations.

In I the technique was illustrated by a calculation for the $\langle 111 \rangle$ split crowdion configuration in Tungsten. The present work extends the calculations to the other five possible interstitial configurations for this metal. In addition to the displacement field calculations, relations are developed for the energy and volume of formation of an interstitial, and results for these properties will also be reported.

In a formal sense the Green's function equations provide a rigorous description of a crystal lattice perturbed by the presence of a defect. In attempting to apply the equations to a particular metal however one must in some way evaluate the various parameters arising in the theory. Lacking a precise microscopic theory for these parameters one is virtually forced to proceed somewhat phenomenologically. A basic assumption of the present work is that the crystal energy may be expressed as

the sum of a pairwise central force interaction term and a term depending only on the volume per atom. This model is suggested by pseudopotential theory (Heine and Weaire 1970) where such terms arise from a second order perturbation expansion of the crystal energy. A consequence of the volume dependent term is that the Cauchy relations (see e.g. Johnson 1972), which would be in effect for a model involving pair interactions alone, need not be satisfied.

In numerical calculations two "semi-empirical" interatomic potentials fitted to experimental data for Tungsten have been employed. No attempt was made to ascertain the precise form of the volume dependent term.

In section 2 the determination of the interatomic potentials for Tungsten is discussed. Sections 3, 4, and 5 are devoted respectively to the displacement field, energy of formation and volume of formation. A discussion of the results is given in section 6.

2. INTERATOMIC POTENTIAL

At present no serious attempt has been made to derive an interatomic potential for a transition metal from a microscopic theory. Clearly this would be a formidable task[†]. Instead, a more primitive approach is often taken. One fits a specified function to certain available experimental data and cuts the potential off at a convenient point. For example, the potential may be expressed in terms of several polynomial sections in which the coefficients are parameters to be fit. The latter technique is referred to as the "spline" method. Potential parameters can be determined so as to reproduce such properties as the elastic constants, phonon spectra, defect formation and migration energies and threshold displacement damage energies. The spline method suffers from the drawback that regardless of the number of data one tries to fit the form of the potential cannot be established uniquely.

A spline potential for Tungsten fitting the elastic constants and vacancy formation energy has been developed by Johnson and Wilson (1972). In principle, the phonon spectra contain somewhat more information concerning the interatomic forces than the elastic constants. A potential has therefore been constructed from interatomic force constants fitted to phonon dispersion curves for Tungsten. The force constants were determined from a two neighbor "axially symmetric" model (Lehman et al. 1962). The potential was also adjusted to agree with the

[†]Although difficult this approach may become feasible with the development of Harrison's d-band metal pseudopotential (Harrison 1969, Moriarty 1972).

formation energy and at short range connects smoothly to a Born-Mayer potential[†]. The parametrization of this potential (referred to as I) is given in Table 1. Potential I and the Johnson and Wilson potential (labeled II) are plotted in Figure 1.

Two important differences between these potentials are worth noting. Potential I unlike potential II has a positive slope at the nearest neighbor position indicating an attractive interaction. Furthermore, a point of inflection or "kink" appears in potential I between the first and second neighbor. Further comment on this feature is made in sections 3 and 6.

The depth of the minimum in potential I is somewhat greater than that of potential II largely because of an assumed vacancy formation energy of 3.6 ev (Gripshover et al. 1970) as opposed to the value of 1.8 ev used by Johnson and Wilson (1972).

[†] In fitting the vacancy formation energy the term E_d in equation (4.6) was neglected. The Born-Mayer parameters were obtained by an extrapolation using Brinkman's scaling formulae (1962) of values determined for iron by Erginsoy, Vineyard and Englert (19

3. DISPLACEMENT FIELD

Displacement fields have been calculated for the six equilibrium configurations of self interstitial atoms in Tungsten. Displacements of atoms in the "perturbed space" including the interstitial core are determined from the relation (equation (2.14) in I)

$$u^r = g^r f^r \quad (3.1)$$

u^r , g^r and f^r are the reduced space displacement, Green's function and force respectively. The Green's function is evaluated from the relation (equation (2.15) in I)

$$g^r = (1 - g^{or} \delta \phi^{pr})^{-1} g^{or} \quad (3.2)$$

where g^{or} is the zeroth order reduced space Green's function and $\delta \phi^{pr}$ is the projection onto the reduced space of the change in the dynamical matrix due to the presence of the interstitial. The explicit formulae used in the evaluation of these quantities are given in I.

The designated interstitial core atoms for each of the six configurations are listed in Table 2. Also listed in this Table are the corresponding symmetry groups (labeled as in Jones 1960), numbers of atoms in the cores and perturbed spaces and reduced space dimensions n_r . The core consists of atoms displaced from their normal lattice sites by $\approx 0.07a$ (where a is half the lattice constant) and the remainder of the perturbed space includes atoms interacting directly with the core.

In the case of the $\langle 110 \rangle$ split interstitial, for example, $n_r = 50$. The evaluation of g^r by equation (3.2) in this case calls for the inversion of a 50×50 matrix, a task routinely per-

formed on a computer. This was the largest matrix requiring inversion in the present calculations.

Once the perturbed space equations have been solved displacements for the rest of the lattice can be evaluated from the relation (equation 2.13 in I)

$$U = G_{21}^0 f^* \quad (3.3)$$

Displacements calculated for the first twenty shells of atoms surrounding the $\langle 110 \rangle$ split and $\langle 111 \rangle$ activated crowdion are listed in Tables 3 and 4 respectively[†].

Difficulties were encountered in the calculations for the $\langle 100 \rangle$ split and octahedral interstitials in the case of potential I. For these configurations certain pairs of atoms are separated by a distance located near the "kink" in this potential. Since the Green's function method is based on an expansion of the crystal energy to harmonic order, a vanishing of the second derivative can give rise to spuriously large calculated displacements. In order to avoid this problem, we have adopted the somewhat ad-hoc approximation of setting equal to zero the matrix elements in $\delta\phi^P$ involving the 511 shell for the octahedral and the 400 and 511 shells for the $\langle 100 \rangle$ split interstitial. The relative separation of the 511 and 311 atoms and the 400 and 200 atoms for the above mentioned configurations are located near the kink in potential I.

[†]Results for the tetrahedral, octahedral and $\langle 100 \rangle$ split configuration will be furnished by the authors upon request.

4. ENERGY OF FORMATION

As discussed in the introduction we assume that the crystal energy may be expressed in the form

$$\Phi = \frac{1}{2} \sum_{\mathbf{r}_i, \mathbf{r}_j} V(|\mathbf{r}_i - \mathbf{r}_j|) + NV(\Omega_0) \equiv v + NV \quad (4.1)$$

Here $V(\Omega_0)$ depends on the average atomic volume $\Omega_0 = \Omega/N$ and $v(r)$ is the interatomic potential. Making use of the equilibrium condition

$$\frac{\partial \Phi}{\partial \Omega} = 0$$

one can express the energy of interstitial (or vacancy) formation entirely in terms of pair interactions (Chang and Falicov 1971). If $\Phi_p(N, \Omega)$ is the energy of a perfect crystal and $\Phi_i(N, \Omega_i)$ is that for a crystal containing an interstitial, the formation energy may be written

$$E_f^i = \Phi_i(N, \Omega_i) - \Phi_p(N, \Omega).$$

Since

$$\Phi_p(N, \Omega_i) = \Phi_p(N, \Omega) + O\left(\frac{1}{N}\right),$$

where the final term, being of order $\frac{1}{N}$, can be neglected, one can write

$$\begin{aligned} E_f^i &= \Phi_i(N, \Omega_i) - \Phi_p(N, \Omega_i) \\ &= v_i(N, \Omega_i) - v_p(N, \Omega_i) \end{aligned}$$

The volume term therefore cancels and only the pair term need be considered.

E_f^i may be divided into three contributions:

$$E_f^i = E_c^i + E_d + E_s \quad (4.2)$$

The origin of these terms may be understood with the help of Fig. 2. Consider a three step process in which a. an atom is removed to infinity from a kink site on the surface; b. the crystal is expanded from a volume $(N-1)\Omega_i/N$ to Ω_i ; c. the atom at infinity is placed at an interstitial site and the surrounding lattice is allowed to relax. The intermediate stages are represented diagrammatically as in a recent note by Hirth (1972). The three terms in equation (4.2) correspond to the steps mentioned above.

The configuration energy E_C^i is defined as

$$E_C^i = v_i(N, \Omega_i) - v_p(N-1, \Omega_i) . \quad (4.3)$$

In a Green's function calculation it is convenient to approximate the first term on the right-hand side of this equation as

$$v_i = v_{i0} + E_R$$

where v_{i0} corresponds to the initial configuration of the interstitial core (reference I) and the relaxation energy E_R may be expressed as[†]

$$\begin{aligned} E_R &= -\frac{1}{2} \sum_l \vec{F}(l) \cdot \vec{u}_l \\ &= -\frac{1}{2} \sum_{i=1}^{n_r} \vec{f}_i^T \vec{u}_i^T \end{aligned} \quad (4.4)$$

The reduced space forces $\vec{f}_i^T$ and displacements $\vec{u}_i^T$ are defined in I.

The second term in equation (4.2), which we refer to as the

[†]Referring to equation (2.1) in I one has $v_i = v_{i0} - Fu + \frac{1}{2}u\phi u$. With the substitution of equation (2.2) this becomes $v_i = v_{i0} - \frac{1}{2}Fu$ which leads to equation (4.4).

dilatational energy, is given by

$$\begin{aligned} E_d &= v_p(N-1, \Omega_i) - v_p(N-1, \frac{N-1}{N} \Omega_i) \\ &= \frac{1}{6} \sum_k v'(R_k) R_k, \end{aligned} \quad (4.5)$$

where the prime denotes differentiation. This term is the change in the pair energy resulting from an expansion of the crystal by one unit cell.

Finally E_s is given by

$$E_s = v_p(N-1, \frac{N-1}{N} \Omega_i) - v_p(N, \Omega_i).$$

This term arises from breaking the "bonds" of an atom at the crystal surface. It is not defined unless the surface configuration is known. Commonly, one approximates $E_s \approx -\frac{1}{2} \sum_k v(R_k)$. E_s should not be identified with the sublimation energy since the volume term V also contributes to the latter.

Performing a similar derivation for a vacancy one arrives at a formation energy of

$$E_f^V = E_c^V - E_d - E_s \quad (4.6)$$

where $E_c^V = v_v(N-1, \Omega_v) - v_p(N, \Omega_v)$ is the vacancy configuration energy. Adding equation (4.2) to equation (4.6) one obtains

$$E_f^{iv} = E_f^i + E_f^V = E_c^i + E_c^V \quad (4.7)$$

E_f^{iv} is the stored energy for a Frenkel pair in the limit of large separation.

All three terms appearing in equation (4.2) are somewhat sensitive to the form of the interatomic potential. In particular the truncation of $v(r)$ at short range, as in potentials

I and II, may result in large errors in the evaluation of E_d . If one considers, for example, a potential exhibiting Friedel oscillations at large distances, then E_d contains a lattice sum of the form

$$\sum_{\mathbf{R}_\ell} \frac{\sin k_F R_\ell}{R_\ell^2}$$

which is known to converge very slowly (Shaw 1968). E_s is also a difficult term to deal with because it depends on the surface configuration, which is not well defined.

The most interesting term in equation (4.2) is E_c^i since it determines the relative stability of different possible interstitial configurations. Table 5 lists calculated values of E_c^i for six interstitial configurations. For potential I the $\langle 110 \rangle$ split and $\langle 100 \rangle$ split, having almost equal energies, are the most stable configurations. In the case of potential II the tetrahedral configuration has the lowest energy.

One notes that the configuration energies for potential II are considerably higher than those for potential I. This is largely a consequence of the relative values of $v(r)$ around $r \approx 1.5a$ (see Fig. 1), the approximate separation between interstitials and their nearest neighbors.

The wide divergence of the results for the two potentials illustrates the sensitivity of such calculations to the exact form of the potential. This sensitivity was previously noted by DePino, Doran and Beeler (1970) who investigated the effect of the cutoff point of the potential on the relative stability of different configurations.

Using the value of E_C^i for the low energy configuration in conjunction with equation (4.7) one can estimate the stored energy for a Frenkel pair. One obtains 9.1 ev and 11.1 ev respectively for potentials I and II, not unreasonable values for Tungsten.

5. VOLUME OF FORMATION

The volume of point defect formation is determined by the condition that the energy of the crystal containing the defect be stationary with respect to a uniform volume expansion. Consider a dilatation in which the l^{th} atom is displaced $\Delta \vec{R}_l = (\vec{R}_l - \vec{R}_i)\delta$ where δ is the dilatation parameter[†] and $\vec{R}_i$ is the center of mass of the defect, in this case an interstitial. At the equilibrium volume Ω_i of an N atom crystal one has

$$\frac{\partial \phi_i(N, \Omega_i)}{\partial \delta} = \frac{\partial v_i(N, \Omega_i)}{\partial \delta} + N \frac{\partial V(\Omega_i/N)}{\partial \delta} = 0. \quad (5.1)$$

It is convenient to write v_i in the form

$$\begin{aligned} v_i(N, \Omega_i) &= v_p(N-1, \Omega_i) + E_c^i \\ &= (N-1) \tilde{v}(\Omega_i/(N-1)) + E_c^i. \end{aligned}$$

The derivative of this expression can be written to first order in δ as

$$\frac{\partial v_i(N, \Omega_i)}{\partial \delta} = (N-1) \{ 3\tilde{v}'(\Omega_0)\Omega_0 + 9\tilde{v}''(\Omega_0)\Omega_0^2\delta \} + \frac{\partial E_c^i}{\partial \delta} \quad (5.2)$$

where the primes denote differentiation and $\Omega_0 = \Omega/N$. The final term in equation (5.2) can be approximated by

$$\begin{aligned} \frac{\partial E_c^i}{\partial \delta} &\approx -\sum_{\alpha} F_{\alpha}^*(l) (R_{l\alpha} - R_{i\alpha}) \\ &= \sum_{j=1}^{n_r} f_j^{r*} r_j^r = -\sum_{\alpha} G_{\alpha\alpha}^i \end{aligned} \quad (5.3)$$

[†]One can generalize the following derivation by considering a tensor dilatation $\delta_{\alpha\alpha}$ but the final result, i.e. equation (5.6) is unchanged.

where

$$r_j^r = \sum_{l\alpha} \psi_{\alpha}^j(l) (R_{l\alpha} - R_{i\alpha})$$

and

$$f_j^{r*} = \sum_{l\alpha} \psi_{\alpha}^j(l) F_{\alpha}^*(l);$$

the quantities F^* and ψ are defined in I. In equation (5.3) a term involving the difference between lattice pair interactions in the distorted and undistorted crystals has been neglected. This term may be made as small as one desires by choosing a large enough interstitial core region. The quantity $G_{\alpha\alpha}^i$ is the so-called strength tensor and is related to the displacement field far from the defect (Hardy 1968). One may note, incidentally, that core atoms do not contribute to the summation in equation (5.3)[†].

The final derivative in equation (5.1) may be written to first order in δ as

$$\frac{\partial V(\Omega_i/N)}{\partial \delta} = 3V'(\Omega_0)\Omega_0 + 3V''(\Omega_0) (3\delta - \frac{1}{N}) \Omega_0^2 \quad (5.4)$$

Substituting equations (5.2), (5.3) and (5.4) into equation (5.1) and recognizing that $\tilde{V}'(\Omega_0) + V'(\Omega_0) = 0$, one obtains

[†]This may be seen as follows. Substituting equation (2.4) into (2.1) of I, one has $\phi = \phi_0 - Fu + \frac{1}{2}u(\phi^0 - \delta\phi)u$. For core atoms

$-\frac{\partial \phi}{\partial u_l} = F_l - (\delta\phi u)_l = F_l^* = 0$. Thus the "Kanzaki force" on core atoms is zero.

$$\begin{aligned} -\text{Tr } G^i &= 3\tilde{V}'(\Omega_0)\Omega_0 + 3V''(\Omega_0)\Omega_0^2 \\ + 9N\Omega_0^2 \delta (\tilde{V}''(\Omega_0) + V''(\Omega_0)) &= 0. \end{aligned}$$

Solving for δ , one gets

$$\delta = \frac{\text{Tr } G^i + 3\tilde{V}'\Omega_0 + 3V''\Omega_0^2}{9N\Omega_0 K} \quad (5.5)$$

where $K \equiv \Omega_0(\tilde{V}'' + V'')$ is the bulk modulus. Using this result one can write the volume of formation as

$$\begin{aligned} \Omega_f^i &= \Omega_i - \Omega = \Omega(3\delta - \frac{1}{N}) \\ &= \frac{\frac{1}{3} \text{Tr } G^i + \tilde{V}'\Omega_0 + V''\Omega_0^2}{K} - \Omega_0 \quad (5.6) \end{aligned}$$

The corresponding result for vacancies is

$$\Omega_f^v = \frac{\frac{1}{3} \text{Tr } G^v - \tilde{V}'\Omega_0 - V''\Omega_0^2}{K} + \Omega_0 \quad (5.7)$$

Adding equations (5.6) and (5.7) one obtains the volume of formation of Frenkel pairs:

$$\Omega_f^{iv} = \frac{\text{Tr}(G^v + G^i)}{3K}$$

One may note that for a crystal interacting by pair forces alone (i.e. $V=0$) the simpler results

$$\Omega_f^{(i,v)} = \frac{\text{Tr } G^{(i,v)}}{3K} \quad (-,+) \Omega_0$$

hold.

Numerical values of $\text{Tr } G^i / (3K\Omega_0) - 1$ obtained for both

Tungsten potentials are presented in Table 5. Unfortunately the quantities $\tilde{v}'(\Omega_0)$ and $\tilde{v}''(\Omega_0)$ may not be directly evaluated since the volume dependence of $v(r)$ is not known.

6. DISCUSSION

The present paper, in conjunction with I, explores the application of lattice Green's functions to static properties of self-interstitial atoms in metals. Tungsten has been considered as a specific example, however the methods discussed are in no way restricted to this metal. In particular, an interstitial in an fcc metal would be somewhat simpler to deal with than the case considered here. The lattice distortion for such a defect is somewhat less severe than for its bcc counterpart; this results in a smaller interstitial core size and consequently less computation. The extension of the present methods to solute interstitials is also straightforward, assuming the impurity-host interaction is known.

In attempting to assess the validity of a particular numerical calculation, two types of errors should be considered. On one hand there are errors in the computational method and on the other errors due to the inaccuracy in the interatomic potential. Computational errors arise from the neglect of anharmonic terms in the crystal energy. In principle, anharmonic corrections can be made as small as desired by choosing a large enough interstitial core[†]. How large a core is necessary in a given situation is difficult to determine in a systematic way. Inspection and trial and error, however, are usually sufficient to reveal which atoms should be included

[†]As described in I, core atoms are treated formally as defects and anharmonic corrections are already included for these atoms.

within the core. A rough estimate of the error in the displacement field calculated for a given interstitial core may be obtained by repeating the calculation for a core augmented by one of two shells of atoms. Incidentally, the size of the core necessary to achieve a certain accuracy in the displacement field may not be the same as that required to achieve a similar accuracy in the energy and volume of formation.

Anharmonic corrections may pose serious difficulties if the interatomic potential is not a smooth and well behaved function. In particular, if the equilibrium spacing of certain pairs of atoms lies near a point of inflection of the potential large errors may result. As mentioned in section 3 such a situation arises when potential I is applied to the octahedral and $\langle 100 \rangle$ split configurations.

The other type of error derives from the inaccuracy in the assumed form of the interatomic potential. As remarked earlier the configuration energy is particularly sensitive to the exact shape of the potential. In the case of transition metals such as Tungsten the potential has not been established with any certainty.

It is worth considering whether a more carefully fitted spline would remove some of the ambiguity in the potential function. It is possible of course to attempt to fit a larger number of data than was done in deriving the curves appearing in Fig. 1. However it is doubtful that this would be an improvement. For one thing, the manner in which a potential should be fitted to properties which are related to

it in a complicated way, such as the threshold energy for radiation damage, the equilibrium crystal structure, etc. is not easy to determine. Furthermore, few properties are sensitive to the potential at distances between lattice interatomic spacings, e.g. between the first and second neighbors. The question of where to cut the potential off also poses a serious problem.

A more fundamental question is whether the concept of a two body central force potential is valid for a transition metal. The kink appearing in potential I between the first and second neighbors may be the product of a "forced fit" rather than an intrinsic feature of the potential. The appearance of this kink may be an indication that the bonding in Tungsten is directional and that therefore an angular dependence should be introduced into the potential. The kink, however, cannot be eliminated simply by considering a larger number of neighbors within the axially symmetric (central force) model. Least squares force constant fits to the phonon spectra show the kink persisting even for an eight neighbor model. Incidentally, phonon spectra for Molybdenum (Woods and Chen 1964), Niobium (Nakagawa and Woods 1963) and Tantalum (Woods 1964) seem to indicate the presence of a kink also for these metals.

In contrast to the situation for the energy and volume of formation, the calculated displacement field is relatively insensitive to the interatomic potential. This may be seen by comparing the displacements corresponding to the two potentials, listed in Tables 3 and 4.

At present there is no direct experimental evidence as to which of the possible interstitial configurations is the most stable. Because of the sensitivity of energy calculations to the interatomic potential and the difficulty in establishing the precise form of the latter, theory cannot provide a firm answer to this question either. The relative insensitivity of the displacement field calculations to the potential may be helpful in this regard. Such calculations may enable us to interpret certain experiments which relate directly to the lattice distortion. It is known that interstitials give rise to characteristic "contrast" effects when observed in the field ion microscope (FIM). Recently a model has been proposed (Seidman and Lie 1972) which relates this contrast to the lattice strain field surrounding an interstitial. The amenability of Tungsten to FIM observation was one motivation for the present study. Another property of considerable interest is X-ray diffuse scattering (e.g. Eisenriegler 1971). This weak scattering occurring between Bragg peaks is related to the Fourier transform of the lattice distortion present in a crystal. Both FIM and X-ray measurements have some promise of eventually revealing the stable configuration of an interstitial.

ACKNOWLEDGMENT

We are grateful to Professor B. N. Brockhouse for providing us with phonon dispersion data for Tungsten.

This work was supported by the United States Atomic Energy Commission, under Contracts AT(11-1)-3158, and AT(11-1)-3171. Additional support was received from the National Science Foundation through the use of the technical facilities of the Materials Science Center, Cornell University.

REFERENCES

- BENEDEK, R., and HO, P. S., 1973, J. Phys. F, to be published.
- BRINKMAN, J. A., 1962, in Radiation Damage in Solids, edited by Billington, D. S., (New York: Academic) 830-859.
- CHANG, R. and FALICOV, L., 1971, J. Phys. Chem. Solids 32, 465-473.
- DE PINO, A. JR., DORAN, D. G. and BEELER, J. R. JR., 1970, RADIATION EFFECTS 3, 23-31.
- EISENRIEGLER, E., 1971, CRYSTAL LATTICE DEFECTS 2, 181-195.
- ERGINSOY, C., VINEYARD, G. H. and ENGLERT, A., 1964, Phys. Rev. 133, A595-A606.
- GRIPSHOVER, R. J., KHOSHNEVISAN, M., ZETTS, J. S. and BASS, J., 1970, Phil. Mag. 21, 757-777.
- HARDY, J. R., 1968, J. Phys. Chem. Solids 29, 2009-2014.
- HARRISON, W. A., 1969, Phys. Rev. 181, 1036-1053.
- HEINE, V. and WEAIRE, D., 1970, in Solid State Physics, Ehrenreich, H., Seitz, F. and Turnbull, D. eds. (New York: Academic) Vol. 24, pp. 249-463.
- HIRTH, J. P., 1972, in Interatomic Potentials and Simulation of Lattice Defects, Gehlen, P. C., Beeler, J. R. Jr., and Jaffee, R. I. eds. (New York: Plenum) p. 456.
- JOHNSON, R. A., 1972, Phys. Rev. B6, 2094-2100.
- JOHNSON, R. A. and WILSON, W. D., 1972, in Interatomic Potentials and Simulation of Lattice Defects, Gehlen, P. C., Beeler, J. R. Jr. and Jaffee, R. I., eds (New York: Plenum) pp. 301-319.
- JONES, H., 1960, The Theory of Brillouin Zones and Electronic States in Crystals (Amsterdam: North Holland Publishing Co.)
- LEHMAN, G. W., WOLFRAM, T. and DE WAMES, R. E., 1962, Phys. Rev. 128, 1593-1599.
- MORIARTY, J. A., 1972, Phys. Rev. B6, 1239-1252.
- NAKAGAWA, Y. and WOODS, A. B. D., 1963, Phys. Rev. Lett. 11, 271-274.
- SEIDMAN, D. N. and LIE, K. H., 1972, Acta Met. 20, 1045-1059.

SHAW, R. W. JR., 1968, Thesis, Stanford Univ., unpublished.

WOODS, A. D. B. and CHEN, S. H., 1964, Solid State Comm. 2, 233-237.

WOODS, A. D. B., 1964, Phys. Rev. 136, A781-A783.

Figure 1.

FORMATION OF AN INTERSTITIAL

FIGURE CAPTIONS

1. Interatomic potentials for Tungsten. Positions of first three nearest neighbors are indicated.
2. Cycle representing the formation of an interstitial. P and I refer to a perfect crystal and a crystal containing an interstitial respectively. Ω_i is the equilibrium volume of an N atom crystal containing an interstitial while Ω is that for a perfect N atom crystal. In step a an atom taken from a surface kink is removed to infinity. Since the surface plays no further role the boundary is represented as a circle for steps b and c. In step b the crystal is expanded from a volume $(N-1)\Omega_i/N$ to Ω_i . In step c the atom from infinity is placed at an interstitial site and the surrounding lattice allowed to relax. E_s , E_d and E_c are the energies associated with steps a, b and c respectively.

TABLE 1. PARAMETRIZATION OF POTENTIAL 1 FOR TUNGSTEN.

The potential is expressed in terms of four polynomial sections, each of the form

$$v(r) = D_0^j + D_1^j (r-R_j) + D_2^j (r-R_j)^2/2 + D_3^j (r-R_j)^3/6$$

$$+ D_4^j (r-R_j)^4/24 \text{ for } r \text{ in the range } x_j < r < x_{j+1}.$$

The derivatives D^j , the expansion points R_j , and the "knot" points x_j are given below. $v(r)$ is in eV and r in units of half the lattice constant.

j	R_j	x_j	D_0^j	D_1^j	D_2^j	D_3^j	D_4^j
1	1.40	1.25	1.4261	-19.475	121.27	-1270.9	40392
2	1.73205	1.45	-.61708	1.0064	10.187	-232.01	819.21
3	2.00	1.866	-.43723	.39027	7.7963	106.59	-785.77
4	2.25	2.10	-.07826	1.3307	-11.491	-48.42	1667.0

TABLE 2. Composition of interstitial core and perturbed space for six configurations in tungsten. Symmetry groups are labeled as in ref. 11. n_s is the number of atoms in a given shell. n_c and n_p are total numbers of atoms in the core and perturbed space respectively while n_r is the dimension of the reduced space.

CONFIGURATION	<110>SPLIT		<111>SPLIT		<111>ACTIVATED		<100>SPLIT		OCTAHEDRAL		TETRAHEDRAL	
SYMMETRY GROUP	N		L		L		X		X		W	
CORE SHELLS	SHELL	n_s	SHELL	n_s	SHELL	n_s	SHELL	n_s	SHELL	n_s	SHELL	n_s
	xx0	2	xxx	2	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	1	x00	2	100	1	$10\frac{1}{2}$	1
	111	4	111	2	111	2	200	2	200	2	111	4
	200	4	222	2	222	2	111	8	111	4	311	8
	202	8	333	2	333	2	222	8	311	8	222	8
	222	4	444	2	444	2	311	8	400	2	133	4
							020	4	222	8	$11\bar{1}$	4
									220	8	113	4
n_c	22		10		9		32		33		33	
n_p	116		72		65		138		119		109	
n_r	50		26		23		33		29		45	

TABLE 3. Atomic displacements $\Delta \vec{r}_\ell = \vec{r}_\ell - \vec{R}_\ell$ for $\langle 110 \rangle$ split interstitial in Tungsten. I and II refer to potentials plotted in figure 1. (units:a)

ℓ	I			II		
	Δr_1	Δr_2	Δr_3	Δr_1	Δr_2	Δr_3
xx0	.545	-.545	.000	.537	.537	.000
111	.060	.060	.370	.112	.112	.315
200	.106	-.006	.000	.111	.048	.000
202	.059	-.020	.054	.050	-.020	.036
222	.075	.075	.070	.105	.105	.086
113	.012	.012	.033	.011	.011	.050
333	.031	.031	.031	.043	.043	.037
111	-.005	.005	.038	-.032	.032	-.007
311	.023	.019	.021	.039	.030	.024
002	.000	.000	.003	.000	.000	-.041
220	.023	.023	.000	-.006	-.006	.000
222	.006	-.006	.014	-.007	.007	.000
220	-.004	.004	.000	-.026	.026	.000
400	.011	.006	.000	.034	.012	.000
113	-.003	.003	.021	.006	-.006	.000
422	.027	.013	.013	.041	.019	.015
224	.012	.012	.029	.016	.016	.034
331	.021	.021	.006	.023	.023	-.001
313	.025	.011	.028	.026	.011	.026
313	.020	-.010	.025	.015	.007	.017

TABLE 4. Atomic displacements $\Delta \vec{r} = \vec{r}_i - \vec{R}_i$ for $\langle 111 \rangle$ activated crowdion (located $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ in Tungsten. I and II refer to potentials plotted in figure 1. (units:a)

i	I			II		
	Δr_1	Δr_2	Δr_3	Δr_1	Δr_2	Δr_3
111	.371	.371	.371	.375	.375	.375
222	.250	.250	.250	.264	.264	.264
333	.139	.139	.139	.167	.167	.167
444	.081	.081	.081	.103	.103	.103
555	.044	.044	.044	.050	.050	.050
200	.018	.002	.002	.047	.032	.032
220	.008	.008	.006	-.004	-.004	-.032
311	.010	.018	.018	.049	.043	.043
331	.048	.048	.037	.038	.038	.008
666	.024	.024	.024	.028	.028	.028
422	-.016	.054	.054	.059	.046	.046
442	.049	.049	.040	.046	.046	.031
553	.037	.037	.039	.064	.064	.041
355	.026	.039	.039	.022	.041	.041
644	.043	.026	.026	.056	.030	.030
$\bar{1}11$	-.018	-.002	-.002	-.047	-.031	-.031
$2\bar{2}0$	-.007	-.002	-.005	-.005	-.003	-.005
$\bar{1}13$	.007	.005	.002	.004	.005	.003
$11\bar{3}$	-.010	-.010	-.002	-.012	-.012	-.010
$\bar{2}22$	.004	.000	.000	-.003	-.004	-.004

TABLE 5. NUMERICAL RESULTS FOR CONFIGURATION ENERGY AND
 PARAMETER $\text{Tr } G^i / (3K\Omega_0) - 1$ ENTERING FORMATION
 VOLUME. I and II refer to potentials plotted
 in figure 1. E_C^i is in eV.

CONFIG.	E_C^i		$\text{Tr } G^i / (3K\Omega_0) - 1$	
	I	II	I	II
<110> SPLIT	1.52	10.98	1.19	1.48
<111> SPLIT	2.84	12.19	.49	1.67
<111> ACTIVATED	2.86	12.32	.42	1.53
<100> SPLIT	1.50	13.77	.23	1.38
OCTAHEDRAL	1.98	9.12	-.04	1.29
TETRAHEDRAL	2.47	7.50	1.27	1.73