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by

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DIRECT OBSERVATION OF THE VACANCY STRUCTURE OF A (220) PLATELET
IN AN ION-IRRADIATED PLATINUM-4.0 at.% GOLD ALLOY[†]

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ABSTRACT

A detailed field-ion microscope (FIM) study has been made of the vacancy structure of a (220) platelet created by a single 30 keV W^+ ion in a platinum-4.0 at.% gold alloy; the specimen was maintained at 40 K (below substage II_B) during the in-situ irradiation at $\sim 2 \times 10^{-9}$ torr. Prior to the pulsed field-evaporation dissection of the specimen at 40 K it was warmed isochronally to 100 K (above substage II_C). The (220) platelet was found to consist of 31 vacant lattice sites, lying in four (220) planes, and clustered in a disc-shaped region which is ~ 20 Å in diameter. If only first nearest-neighbor lattice sites are considered then the distribution of cluster sizes is as follows: (1) two monovacancies; and (2) one jumbo vacancy cluster containing 29 vacancies. The range of the vacancy concentration within the (220) vacancy platelet is ~ 35 to 44 at.%. Employing the modified Kinchin-Pease equation it was calculated that the displacement efficiency (κ) for this platelet is 0.12. It is suggested that the prismatic dislocation loops lying on {220} type planes, observed by transmission electron microscopy, in ion or fast-neutron irradiated platinum can form as a result of the direct collapse of {220} type vacancy platelets.

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§ INTRODUCTION

The point-defect structure of the primary state of damage of irradiated metals can, at present, only be studied experimentally by the field-ion microscope (FIM) technique. The FIM technique provides us with an exact picture of the arrangement of vacant lattice-sites and self-interstitial atoms (SIAs) within and around a depleted zone created by a single primary knock-on atom (Seidman 1973 and 1976). The present paper represents an extension of our earlier research on the body-centered cubic metal tungsten (Beavan, Scanlan and Seidman 1971, Wilson and Seidman 1973) to a face-centered cubic platinum-4.0 at.% gold alloy. There is earlier qualitative work on depleted zones in fast-neutron irradiated platinum by Attardo and Galligan (1966 and 1967) and Inal and Galligan (1970); the main emphasis in this work was in determining size distributions whereas our emphasis is on the spatial distribution of vacant lattice sites within and around individual depleted zones.

In the research on tungsten we studied the point-defect structure of depleted zones created at both 18 K (Stage I) and 473 K (near the top of Stage II); see Schilling, Sonnenberg and Dibbert (1972) for a discussion of Stage II in the Pt(Au) system. The work presented here describes the vacant lattice-site structure of a depleted zone that had collapsed into a four-layer vacancy platelet on a (220) plane. The (220) vacancy platelet was created in the Pt-4.0 at.% Au alloy by a single 30 keV W^+ ion at 40 K (below substage II_B); the specimen was subsequently annealed to 100 K (above substage II_C) prior to its examination at 40 K. The (220) vacancy platelet represents an energy state that is intermediate in energy between a three-dimensional compact vacancy cluster and a dislocation loop. The possibility of stable multi-layer vacancy platelets does not seem to have been considered in the theoretical literature on this subject. It is suggested on the basis of our observation of this platelet that prismatic dislocation loops, observed in trans-

mission electron microscopy studies of ion or fast-neutron irradiated Pt, can form directly from the collapse of vacancy platelets on {220} type planes. And that the vacancy supersaturation within a platelet required for collapse into a dislocation loop can be exceedingly large. Finally, we present, for the first time, the application of the OR TEP program (Johnson 1965 and 1970) to provide a stereographic drawing of the vacancy platelet.

§2. EXPERIMENTAL DETAILS

2.1. Specimen chemistry and preparation

The Pt-4.0 at.% Au alloy was prepared at Cornell University and the gold concentration was determined to be 4.0 ± 0.3 at.% by the analytical chemistry laboratory of the Materials Science Center and the U.S. Testing Laboratory (see Table I of Chen and Balluffi 1976). The alloy was drawn into 0.13 mm diameter wire and electropolished in a molten salt solution of NaNO_3 and ~20 % by wt. NaCl, maintained at 350°C, to remove any surface contamination. The wires were next annealed by resistively heating them in air at ~1400 K and then air quenched by rapidly terminating the heating current. Sharply-pointed FIM specimens were prepared by the standard electropolishing-technique (Müller and Tsong 1969) at 3 to 4 Vdc, in the above described molten salt-solution, at 623 K. The procedure consisted of dipping a wire specimen, at regular intervals, into the salt bath to a depth of ~5 mm and rapidly removing it after 0.2 sec. Next the FIM specimen was field-evaporated continuously in the FIM at ~125 K and then pulsed field-evaporated at ~70 K to a final end-form at a background pressure of 1×10^{-4} torr Ne.[†]

[†] All pressures reported in this paper have been converted from gauge to real pressure.

2.2. The irradiation procedure

The specimens were irradiated in-situ in a bakeable ultra-high vacuum FIM which is attached to a Hill-Nelson sputtered-metal ion-source via a three-stage differentially-pumped flight-tube (Scanlan, Styris and Seidman 1971). This arrangement allowed for an in-situ irradiation at $\sim 2 \times 10^{-9}$ torr with a pressure of $(2 \text{ to } 5) \times 10^{-6}$ torr argon measured above the diffusion pump which evacuates the ion source. The alloy was irradiated at 40 K with a magnetically analyzed 30 keV W^+ ion beam to a dose of $\sim 1 \times 10^{13}$ ion cm^{-2} and the flux of ions at the specimen position was $\sim 3 \times 10^{10}$ $\text{cm}^{-2}\text{sec}^{-1}$; at this value of the flux the time required to form an adsorbed monolayer was greater than the irradiation period. After the 40 K irradiation the specimen was annealed isochronally to 100 K (Wei and Seidman 1977).

The specimen temperature was monitored with a miniature platinum resistance thermometer (PRT) mounted near the tail of the cryostat. For further details regarding temperature measurement, the sputtered-metal ion-source and the irradiation facility see our earlier publications (Seidman and Scanlan 1971, Scanlan et al. 1971, Pétroff and Seidman 1973, and Wilson and Seidman 1975).

2.3. Data recording system and ciné film analyzer

The neon FIM images were observed with the aid of an internal image-intensification system based on a Galileo 76 mm diameter channel electron-multiplier array (Brenner and McKinney 1970) and the FIM images produced in this manner were recorded on 35 mm film with the aid of an Automax ciné-camera equipped with a 1000 ft. film chamber. The recorded and developed ciné film was analyzed with a Vanguard motion analyzer which is equipped with x-y cross-hairs and a position readout (Scanlan et al. 1969); the motion analyzer was interfaced to a Houston Omnigraphic 200 x-y recorder. This latter feature was extremely useful for

reconstructing the point defect structure of the depleted zone discussed in this paper. Each FIM image was recorded after a field-evaporation pulse had been initiated; the pulse height and duration were adjusted so that one atom, on the average, was removed per pulse on the (420) plane.

§3. THE ARRANGEMENT OF ATOMS IN THE (75 $\bar{1}$) PLANE

The vacancy platelet (depleted zone A) discussed in this paper was detected in the (75 $\bar{1}$) plane of an FIM specimen with a [100] orientation. This plane is located on the [11 $\bar{2}$] zone inbetween the (220) and (53 $\bar{1}$) planes (see fig. 1a).[†] The interplanar spacing for the (75 $\bar{1}$) plane is $a_0/\sqrt{75}$ ^{*} and there are a series of equally spaced planes between the zeroth plane and the 75th plane.^{**} The atomic arrangement within the (75 $\bar{1}$) plane and the stacking of the (75 $\bar{1}$) planes is a bit complicated, hence we consider this plane in detail.

The crystallography of the (75 $\bar{1}$) plane is not given in Nicholas' atlas (1965), hence we constructed a ball model of a (75 $\bar{1}$) plane according to the procedure developed by Moore and Nicholas (1961). A photograph of this ball model, built on a (200) plane, is shown in fig. 2; the dark balls indicate the atoms in the outermost (zeroth) layer. The visible atoms, within the primitive unit cell, from

[†] The Miller indices (hkl) of the physical planes must be of unmixed parity for an fcc lattice. If the Miller indices are of mixed parity it is a simple matter to convert them to unmixed parity.

^{*} The lattice parameter of the fcc cell is denoted by a_0 ; for the Pt-4.0 at.%. Au alloy $a_0 = 3.921$ Å (Pearson 1958).

^{**} The number of planes in an identity period (N_{hkl}) is given by the expression $N_{hkl} = QQ^*(h^2 + k^2 + l^2)/2$ where Q is one if h, k, l are all odd and Q is 2 if h, k, l are of mixed parity; and Q* is one if h + k + l is even, while Q* is 2 if h + k + l is odd. It is important to note that in making this calculation one must use the Miller indices (hkl) before they have been converted into unmixed parity. We also note that the Jaswon and Dove (1955) statement "that the stacking pattern of the primitive cubic (hkl) planes constitutes a congruence modulo $h^2 + k^2 + l^2$ " is not generally correct.

different layers are indicated by the numbers 1, 2, 3, 4 and 5. The balls marked with an x indicate one $(11\bar{1})$ plane that intersects the $(75\bar{1})$ plane. The ball model was used to determine the primitive mesh and the stacking sequence of planes zero to five. Figure 3 shows the primitive mesh (plane zero) of the $(75\bar{1})$ plane and the positions of the atoms of planes 1 to 5 that project within the primitive mesh; the Appendix and Table 1 give more details concerning fig. 3.[†]

§4. PROCEDURE FOR THE CONSTRUCTION OF A DEPLETED ZONE

In this section the basic procedure used to reconstruct a depleted zone in three-dimensions, from the FIM micrographs, is explained. The steps employed are as follows:

1. The positions of all atoms and vacant sites on the zeroth layer are determined employing the x-y cross-hairs on the motion analyzer in conjunction with the x-y recorder. All the cartesian coordinates are read with respect to a common fiducial mark which had been engraved in the phosphor screen portion of the internal image-intensification system. This procedure eliminated all errors in the positions of atoms caused by the slippage of film in either the ciné camera or the motion analyzer.

2. An atom or vacant site in the zeroth layer is arbitrarily chosen as the origin atom for this layer; the atom labeled $O(0,0,0)$ in fig. 4 is taken to be an origin atom. A schematic diagram showing the positions of the atoms in two successive $(75\bar{1})$ planes, which had been recorded as outlined in step 1, is shown in fig. 4. The atomic sites in the zeroth and first layers are represented by solid black circles and open circles respectively. The vector $\frac{a_0}{2} [\bar{1}1\bar{2}]$ which lies along the intersection of the $(75\bar{1})$ and $(53\bar{1})$ planes was chosen as the u-axis. Similarly,

[†] We have generally followed the scheme of Nicholas (1965) in presenting crystallographic information.

the vector $\frac{a_0}{2} [\bar{2}31]$ which lies along the intersection of the $(75\bar{1})$ and (640) planes was used to determine the vector $\frac{a_0}{2} [\bar{1}23]$ which was taken to be the v-axis (see fig. 4). The vector $(a_0/75)[75\bar{1}]$ which is normal to the $(75\bar{1})$ plane was taken to be the Z-axis (see the Appendix). All of the vectors used so far are in the standard orthogonal coordinate system. Next the coordinates of the atomic sites were indexed with respect to the vectors u, v and OZ $\{(a_0/75)[75\bar{1}]\}$; for example, the sites O, A and B in the zeroth layer have local coordinates $(0,0,0)$, $(1,0,0)$ and $(0,1,0)$ respectively. The origin for the first layer (O') is uniquely assigned to the atomic site which is projected within the unit primitive cell of the zeroth layer (see fig. 4); O'_p denotes the projection of O' onto the zeroth layer then $\vec{O'_p O'} = [00\bar{1}]$. Hence, $\vec{O'_p D} = \vec{O'_p O'} + \vec{O'D} = [00\bar{1}] + [\bar{1}\bar{1}0] = [\bar{1}\bar{1}\bar{1}]$, so that the coordinates of D are $(-1,-1,-1)$ relative to O'_p . The local coordinates of other atomic sites in the first layer, relative to O'_p , are derived in a similar manner. The practical advantage of this local coordinate system is that all the vacant lattice sites have integral coordinates.

3. Finally the coordinates of an atomic site, such as D, relative to the origin O in the zeroth layer, are obtained by adding the shift vector $\vec{t} = [t_x t_y 0]$ to $\vec{O'_p D}$. The shift vector is the projection of $\vec{OO'}$ onto $(75\bar{1})$ and is given by $\vec{t} = (a_0/150)[\bar{6}\bar{1} \ 85 \ \bar{2}]$ (see the Appendix). Extending this procedure the positions of all the atomic sites observed can then be transformed back to an orthogonal coordinate system with O as its origin. In practice all the required transformations were carried out in our laboratory with the aid of a Nova 1220 minicomputer.

§5. RESULTS

In only one out of three ion-irradiated Pt(Au) specimens did we find a mapable and isolated depleted zone in the bulk of a specimen; this specimen had an average radius of curvature of ~ 190 Å. We shall momentarily call this depleted zone DZA; its position in the FIM tip, relative to the two other depleted zones

detected, is shown in fig. 1. It is noted that DZA is located ~ 30 Å down from the initial surface and ~ 90 Å from the irradiated surface of the specimen. Depleted zone B is located near the $(93\bar{1})$ plane and depleted zone C is located near the $(2\bar{2}0)$ plane. Depleted zones B and C were found only one or two interplanar spacings from the irradiated surface of the specimen. The DZA detected in the $(75\bar{1})$ plane was found to consist of 31 vacant lattice sites* clustered in a disc-shaped region, ~ 20 Å in diameter lying near a (220) plane. Thus DZA has the morphology of a vacancy platelet with a (220) habit plane; thus we call it a (220) vacancy platelet.

Figure 5 shows a series of ten FIM micrographs of ten successive $(75\bar{1})$ planes; they were chosen from a total of 1.2×10^3 frames of 35 mm ciné film which were recorded and analyzed in the reconstruction of the (220) vacancy platelet. The $(75\bar{1})$ plane and the surrounding planes are indexed in frame 1; the frame number of the ciné film is located in the lower right-hand corner below each micrograph and the layer number is preceded by the letter n (e.g., n = 1) in the upper left-hand corner above each micrograph. Frames 1, 235, 292 and 898 show atomically perfect planes in layers 1, 3, 4 and 10 respectively; the other frames exhibit $(75\bar{1})$ planes containing vacant lattice-sites. The position of each atom in the $(75\bar{1})$ plane is indicated schematically below each micrograph by a solid black-dot and a vacant lattice-site is indicated by an open circle. Because of the small size of the $(75\bar{1})$ plane we have been forced to include ledge atoms in analyzing the (220) vacancy platelet; a missing atom in the ledge was only counted as a vacant lattice site if no atom was detected in this site during the entire atom-by-atom dissection process of this plane.

* One contrast effect produced by a gold atom is a single dark atom site (Chen and Balluffi 1976); this contrast effect is identical to that of a vacant lattice site. Hence, the 31 vacant sites detected represent an upper limit to the vacancy population in the platelet.

Figure 6 shows a projection of all the vacant sites contained in the vacancy platelet on a (220) plane; this plane was chosen for the projection since the habit-plane of this disc-like agglomerate of vacant lattice sites is very close to the (220) plane. The number(s) associated with the open-circle(s) corresponds to the (220) plane in which the vacant sites reside; the doubly concentric-circle indicates that two vacancies project to the same site. An isometric drawing of the (220) vacancy platelet is shown in fig. 7. The boundary of each slab was constructed by connecting the outermost vacant lattice sites in each slab by straight line-segments; the thickness of each slab is two (220) interplanar spacings (2.77 Å). This isometric representation of DZA shows its plate-like character rather clearly.

Figure 8 exhibits the vacant lattice-sites in the (220) vacancy platelet in a second way. The vacant lattice-sites are projected onto the (0 $\bar{2}$ 0), (200) and (002) planes in figs. 8a, 8b and 8c respectively. The projection onto the (002) plane in fig. 8c shows very clearly that the habit plane is a (220) plane. Figure 8d is a photograph of a ball-model of the (220) vacancy platelet; each ball represents a vacant lattice-site and the surrounding lattice atoms have been omitted for clarity. The photograph in fig. 8d was taken along approximately a $[\bar{1}00]$ direction.

Finally in fig. 9 a computer generated* stereographic drawing of the vacant lattice sites within the (220) vacancy platelet is exhibited. The open circles represent the vacant lattice-sites and the length of the connecting bonds between vacant lattice-sites is equal to the first nearest-neighbor distance ($a_0/\sqrt{2}$) in the fcc lattice. The viewing direction is approximately along an $[0\bar{1}1]$ direction. If only first nearest-neighbors vacant lattice sites are considered then the

* The OR TEP program, developed at the Oak Ridge National Laboratory to provide isometric drawings and stereo-displays of large complex organic and biological molecules, was used to make fig. 9.

distribution of cluster sizes is as follows: (1) two monovacancies; and (2) one jumbo vacancy cluster containing 29 vacancies. This cluster size distribution shows that the (220) vacancy platelet is, indeed, very compact.

The calculation of the vacancy concentration in a depleted zone involves a degree of uncertainty as one must always estimate, in some manner, the number of atoms associated with the depleted zone. We now discuss two procedures for estimating the vacancy concentration (c_v). In the first procedure we employed the number of atomic sites (80) contained within the $\sim 1200 \text{ \AA}^3$ volume of the isometric representation shown in fig. 7; this procedure yielded $c_v \approx 39 \text{ at.}\%$. The value of c_v is lowered to 35 at.% if it is corrected for the gold solute atoms which display the same contrast effect as a vacant lattice site. The second procedure involved calculating c_v in each x-y plane passing through the platelet and then averaging over all x-y planes contained within the depleted zone. The number of atomic sites counted in the calculation of c_v was contained within a rectangle whose borders were determined by the four outermost vacant lattice sites in each x-y plane. This procedure was repeated for the y-z and z-x planes. The average value of c_v obtained in this manner is $\sim 44 \text{ at.}\%$. Thus the possible range of c_v is ~ 35 to $44 \text{ at.}\%$ employing the above two counting procedures.

§6. DISCUSSION

6.1. Probability that the (220) platelet was created by one incident ion

Employing the same geometric argument as the one we used earlier (Beavan, Scanlan and Seidman 1971, Wilson and Seidman 1973) it was estimated that the maximum number of ion hits on the cross-sectional area of the platelet ($\sim 30 \text{ \AA}^2$) was 0.03. This value is an upper bound because the calculation neglects the spread in the range of the incident ions. Since the estimated number of ion hits on the cross-sectional area is approximately 33 times less than unity we

concluded that the vacancy platelet was created by a single incident-ion.

6.2. The number of vacancies in the (220) platelet

The model used most frequently to calculate the number of Frenkel pairs ($\langle v \rangle$) produced by a primary knock-on atom (PKA) is the modified Kinchin-Pease (1955) amorphous solid model. The modified expression for $\langle v \rangle$ is given by: (Robinson and Torrens 1974)

$$\langle v \rangle = \kappa \langle \hat{E} \rangle / 2E_d \quad (1)$$

where $\langle \hat{E} \rangle$ is the average damage energy, κ is the displacement efficiency and E_d is the displacement threshold energy. The quantity $\langle \hat{E} \rangle$ is related to the incident ion energy E_0 by the equation

$$\hat{E} = E_0 - \hat{Q} \quad (2)$$

where $\hat{Q}$ is the total energy lost from a collision cascade through all inelastic processes. In the present situation E_0 is 30 keV, $\hat{Q}$ is 7.26 keV and E_d is 44 eV; the value of $\hat{Q}$ was calculated for the Ta^+ on Au situation employing the recent extensive tabulation of Winterbon (1975). The value of E_d was taken from the tables compiled by Lucasson (1975); this E_d represents an average threshold energy rather than the minimum energy (33 eV) required to produce a displacement in platinum. For the (220) vacancy platelet the value of $\langle v \rangle$ is equal to 31, hence κ is equal to 0.12. This value is considerably less than the value of ~ 0.8 to 0.9 found both from computer simulation studies (Robinson and Torrens 1974) and analytical solutions (Sigmund 1972). This factor of ~ 7 between the calculated and experimental value of κ can be attributed to the following causes: (1) the known straggling of the damage energy (Robinson 1972); (2) fluctuations in the value of $\langle v \rangle$ for a given $\hat{E}$ (Robinson and Torrens 1974); and (3) the enhanced recombination of SIAs and vacancies due to the fact that the specimen was annealed to 100 K (end of substage II_c) prior to its examination at 40 K.

6.3. The diameter of the platelet

An estimate of the expected cascade size in Pt-4.0 at.% Au[†] was made employing the tabulations given by Winterbon (1975). The diameter of the cascade ($D_{\perp}$) was taken to be given by $2(\langle y^2 \rangle)^{1/2}$ (Westmoreland and Sigmund 1970) where $\langle y^2 \rangle$ is the second moment of the damage distribution curve (i.e., the distribution of the fraction of ion energy deposited in atom motion). The value $\langle y^2 \rangle$ was obtained in the following manner: (1) the mean damage depth ($\langle x \rangle$) was calculated (~ 35 A); (2) the relative damage straggling ratio ($\langle \Delta x^2 \rangle / \langle x \rangle^2$) was calculated (0.39); and finally (3) the relative transverse damage straggling ratio ($\langle y^2 \rangle / \langle \Delta x^2 \rangle$) was calculated using the results of steps 1 and 2 (0.51). Employing the above numbers the value of $D_{\perp}$ was determined to be ~ 16 A. This value can be compared to the experimental value of ~ 20 A for the (220) platelet. The experimental and theoretical values are in reasonable agreement^{††}, hence it appears that Westmoreland and Sigmund's method provides a useful approach for obtaining an approximate estimate of the size of a cascade (also see Jenkins and Wilkens 1976).

We further note that the (220) vacancy platelet was located ~ 90 A in from the irradiated surface; this value is a factor of 2.6 greater than the mean damage depth of ~ 35 A and the quantity $[90 - \langle x \rangle]$ A is five times greater than one standard deviation $[(\langle \Delta x^2 \rangle)^{1/2} = 11$ A]. Thus the (220) vacancy platelet lies in the extreme tail end of the damage distribution profile or alternatively it was produced as a result of a dechanneling event; note that the incident ion beam was approximately parallel to the $[00\bar{1}]$ direction (see fig. 1a). In a computer simulation study of depleted zones in copper Robinson and Torrens (1974) have found that the channeled

[†] The present situation of 30 keV W⁺ on Pt-4.0 at.% Au was modeled for 30 keV Ta⁺ on Au.

^{††} The agreement is surprisingly good considering that the specimen was annealed to the top of substage II_C (100 K).

atoms are associated with a reduced number of displacements and a large loss of energy by inelastic processes; thus this may be a fourth possible reason for the small number of vacancies in the (220) platelet and hence the small calculated value of κ in eqn. (1) (see §6.2).

6.4. Stability of the (220) vacancy platelet

The subject of the relative stability of the different possible morphologies of vacancy clusters in quenched or irradiated metals has been the subject of several theoretical treatments (e.g., Sigler and Kuhlmann-Wilsdorf 1966 and Johnson 1967) as well as numerous experimental investigations (e.g., Makin 1966 and Eyre 1973) by a variety of techniques.

The FIM technique has been useful in demonstrating that there are at least three basic morphological types of vacancy clusters in the primary damage state of irradiated metals (Seidman 1976); the simpler primary damage state (a random distribution of Frenkel pairs) produced by MeV electrons is excluded from this categorization. The three basic morphological types are: (1) depleted zones; (2) very compact three dimensional vacancy-clusters or voids; and (3) dislocation loops. The above categorization was based on FIM observations of 10 MeV proton, fast neutron or heavy ion (50-150 keV W^+ , W^{+2} , Zn^+ , Hg^+ , Ar^+ and Xe^+) irradiated specimens of tungsten, iridium and platinum; the irradiations were generally performed at either room temperature or 78 K (see Seidman 1976 for the references from which the above categorization was made). The vacancy concentration stored in the dislocation loops, in the above metals, only represented a small fraction of the total vacancy concentration in the irradiated metals; in the case of tungsten it was ~10%. This is an important result since the transmission electron microscope (TEM) studies of irradiated metals depend heavily on the ability of the vacancy-rich core of a depleted zone to collapse into a dislocation loop; the latter defect is imaged via strain-field contrast in a TEM image (Eyre 1973). With care

it is also possible to observe voids by the TEM technique; although the voids are best observed in an out-of-focus state (Rühle and Wilkins 1975). In conclusion the FIM observations provide a simple explanation for the low values of the yield-factor (Wilkins 1975 and Merkle 1976), determined by the TEM technique, for a number of ion-irradiated metals; that is, of the three basic morphological types only the dislocation loops have been, in general, observed by the TEM experiments. Thus an appreciable fraction of the radiation damage is often in a state of aggregation that is not resolved in the TEM image. This conclusion is corroborated, in the case of platinum, by Schindler's TEM observation (1977) that the yield-factor for platinum irradiated with 60 keV Au⁺⁺ ions is only 0.1.

The (220) vacancy platelet reported and analyzed in this paper must represent an energy state that is intermediate in energy between a three-dimensional compact vacancy cluster (or void) and a dislocation loop. It is interesting to observe that the platelet-like structure exists over four (220) planes (see figs. 7 to 9); this possibility does not appear to have been considered theoretically in the literature.[†] On the theoretical side Johnson (1967) has predicted that a single-layer vacancy-platelet on a {111} plane, in nickel, is stable to collapse into a perfect dislocation loop up to 180 vacancies. While Savino and Perrin (1974) have calculated by a computer simulation technique that a (111) planar vacancy aggregate, in copper, of as few as six vacancies can readily collapse into a more stable configuration. In addition there have been three TEM studies of both fast-neutron irradiated Pt (Ruedl, Delavignette and Amelinckx 1962 and Rühle, Häusserman and Rapp 1970) and 60 keV Au⁺⁺ ion-irradiated (Schindler 1977) platinum. In all three cases prismatic dislocation loops (i.e., with an $\frac{a_0}{2} \langle 110 \rangle$ type Burgers vector) were detected; in Schindler's research (1977) he determined that 90% of the dislocation loops

[†] To the best of our knowledge only the possibility of a single-layer vacancy-platelet had been considered in the theoretical literature.

observed had an $\frac{a_0}{2} \langle 110 \rangle$ type Burgers vector (the remaining 10% of the dislocation loops were Frank loops). Furthermore in unpublished research Schindler (private communication) had determined the habit plane of the prismatic dislocation loops to be of the $\{110\}$ type. Thus we would like to suggest on the basis of our observations in this Pt-4.0 at.% Au alloy and the TEM research on irradiated Pt that the prismatic loops observed, in the TEM studies, formed directly as the result of the collapse of vacancy platelets on the $\{220\}$ type planes. That is, the vacancies need not have first collapsed onto a $\{111\}$ type plane to form a Frank dislocation loop with an $\frac{a_0}{3} \langle 111 \rangle$ type Burgers vector and then unfaulted as a result of the dislocation reaction (Silcox and Whelan 1960)

$$\frac{a_0}{3} [111] + \frac{a_0}{6} [11\bar{2}] \rightarrow \frac{a_0}{2} [110] \quad (3)$$

to form a prismatic dislocation loop.

The final point that we would like to note is the high degree of stability with respect to collapse into a prismatic dislocation loop, of the present vacancy platelet, despite the fact that the local vacancy concentration of 35 to 44 at.% corresponds to a local supersaturation, at 100 K, of $\sim (5 \text{ to } 6) \times 10^{14}$ and therefore to a chemical potential of ~ 1.5 eV per vacancy within the platelet. Thus it would appear that even greater values of the supersaturation, within a platelet, are necessary for it to collapse into a prismatic dislocation loop in the case of platinum.

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REFERENCES

- Attardo, M. J., and Galligan, J. M., 1966, Phys. Rev. Lett., 17, 191.
- Attardo, M. J., and Galligan, J. M., 1967, Phys. Rev., 161, 558.
- Beavan, L. A., Scanlan, R. M., and Seidman, D. N., 1971, Acta Met., 19, 1339.
- Chen, C. G., and Balluffi, R. W., 1975, Acta Met., 23, 931.
- Eyre, B. L., 1973, J. Phys. F: Metal Phys., 3, 422.
- Inal, O. T., and Galligan, J. M., 1970, Acta Met., 18, 1970.
- Jaswon, M. A., and Dove, D. B., 1955, Acta Cryst., 8, 88.
- Jenkins, M. L., and Wilkens, M., 1976, Phil. Mag., 34, 1155.
- Johnson, C. K., 1965 and 1970, Oak Ridge National Laboratory (USA) Report 3794 plus revisions.
- Johnson, R. A., 1967, Phil. Mag., 16, 553.
- Kinchin, G. H., and Pease, R. S., 1955, Rep. Prog. Phys., 18, 1.
- Lucasson, P., 1975, in Intern. Conf. on Fundamental Aspects of Radiation Damage in Metals, edited by M. T. Robinson and F. W. Young, Jr., (National Technical Information Service, Springfield, Virginia), p. 42.
- Makin, M. J., 1966, The Nature of Small Defect Clusters (H. M. Stationary Office, London).
- Merkle, K. L., 1976, in Radiation Damage in Metals, edited by N. L. Peterson and S. D. Harkness (American Society for Metals, Metals Park, Ohio), p. 58.
- Moore, A. J. W., and Nicholas, J. F., 1961, J. Phys. Chem. Solids, 20, 222.
- Müller, E. W., and Tsong, T.-T., 1969, Field-Ion Microscopy (American Elsevier, New York), p. 119.
- Nicholas, J. F., 1965, An Atlas of Models of Crystals Surfaces (Gordon and Breach, New York).
- Pearson, W. B., 1958, A Handbook of Lattice Spacing and Structure of Metals and Alloys (Pergamon Press), Vol. I, p. 821.
- Pétroff, P., and Seidman, D. N., 1973, Acta Met., 21, 323.
- Robinson, M. T., 1972, in Radiation Induced Voids in Metals, edited by J. W. Corbett and L. C. Ianniello, (U.S. Atomic Energy Commission, Washington, D. C.), p. 397.
- Robinson, M. T., and Torrens, I. M., 1974, Phys. Rev. B, 9, 5008.

Ruedl, E., Delavignette, P., and Amelinckx, S., 1962, in Radiation Damage in Solids (IAEA, Vienna), Vol. I, p. 363.

Rühle, M., Häusserman, F., and Rapp, M., 1970, Phys. Stat. Sol., 39, 621.

Rühle, M., and Wilkins, M., 1975, Cryst. Lattice Defects, 6, 129.

Savino, E. J., and Perrin, R. C., 1974, J. Phys. F: Metal Phys., 4, 1889.

Schilling, W., Sonnenberg, K., and Dibbert, H. J., 1972, Radiat. Effects, 16, 57.

Schindler, R., 1977, Dr. rer. nat. Thesis, University of Stuttgart, West Germany.

Scanlan, R. M., Styris, D. L., Seidman, D. N., and Ast, D. G., 1969, Cornell Materials Science Center Report # 1159.

Scanlan, R. M., Styris, D. L., and Seidman, D. N., 1971, Phil. Mag., 23, 1439.

Seidman, D. N., 1973, J. Phys. F: Metal Phys., 3, 393.

Seidman, D. N., 1976, in Radiation Damage in Metals, edited by N. L. Peterson and S. D. Harkness (American Society for Metals, Metals Park, Ohio), p. 28.

Seidman, D. N., and Scanlan, R. M., 1971, Phil. Mag., 23, 1429.

Sigler, J. A., and Kuhlmann-Wilsdorf, D., 1966, in The Nature of Small Defect Clusters, edited by M. J. Makin (H. M. Stationary Office, London), p. 125.

Sigmund, P., 1972, Revue Roum. Phys., 17, 823.

Silcox, J., and Whelan, M. J., 1960, Phil. Mag., 5, 1.

Westmoreland, J. E., and Sigmund, P., 1970, Radiat. Effects, 6, 187.

Wilkins, M., 1975, in Intern. Conf. on Fundamental Aspects of Radiation Damage in Metals, edited by M. T. Robinson and F. W. Young, Jr., (National Technical Information Service, Springfield, Virginia), p. 98.

Wilson, K. L., and Seidman, D. N., 1973, in Defects and Defect Clusters in B.C.C. Metals and Their Alloys, edited by R. J. Arsenault (University of Maryland), p. 216.

Wilson, K. L., and Seidman, D. N., 1975, Radiat. Effects, 27, 67.

Winterbon, K. B., 1975, Ion Implantation Range and Energy Deposition Distributions: Low Incident Energies (IFI/Plenum, New York).

APPENDIX

The vectors $\vec{OR} = \frac{a_0}{2} [0\bar{1}\bar{1}]$, $\vec{OS} = \frac{a_0}{2} [0\bar{1}1]$ and $\vec{w} = \vec{OI} = \frac{a_0}{2} [\bar{1}10]$ define a primitive unit cell in the fcc lattice. The unit mesh exhibited in fig. 3 was shown from the model (fig. 2) to be determined by the vectors $\vec{u} = \vec{OA} = \vec{OR} - \vec{OS} + \vec{OI} = \frac{a_0}{2} [\bar{1}1\bar{2}]$ and $\vec{v} = \vec{OB} = \vec{OS} + \vec{OI} - 2\vec{OR} = \frac{a_0}{2} [\bar{1}23]$; the vectors $\vec{u}$, $\vec{v}$ and $\vec{w}$ also define a primitive unit cell. The shift vector $\vec{t}$ which is the projection of $\vec{w}$ onto the $(75\bar{1})$ plane is given by

$$\vec{t} = \vec{w} - \vec{d},$$

where the vector $\vec{d}$ is perpendicular to the $(75\bar{1})$ plane and has a magnitude equal to the spacing between $(75\bar{1})$ planes. For the $(75\bar{1})$ plane $\vec{d} = \frac{a_0}{75} [\bar{7}51]$ and $\vec{t} = \frac{a_0}{150} [\bar{6}1\ 85\ \bar{2}]$. In fig. 3 $\vec{t}$ lies in the $(75\bar{1})$ plane and it connects 0 with the projection of 1 in the $(75\bar{1})$ plane; similarly the vector $2\vec{t}$ connects 0 with the projection of 2 in the $(75\bar{1})$ plane. The positions of atoms A and B and 1 to 5 relative to the cubic axes and also relative to 0 X Y Z were calculated following the approach developed by Nicholas (1965) and are listed in Table 1. This crystallographic information is given for completeness, since it is not available elsewhere in the literature for the $(75\bar{1})$ plane.

Table 1: Table of Atomic Positions for the $(75\bar{1})$ Plane

Atom	Co-ordinates of Position*								
	Relative to Cubic Axes			Relative to O X Y Z					
				$/\sqrt{6}$	$/\sqrt{450}$	$/\sqrt{75}$			
A	-1	1	-2	6	0	0	2.4495	0	0
B	-1	2	3	-3	75	0	-1.2247	3.5355	0
1	-1	1	0	2	24	-2	0.8165	1.1314	-0.2309
2	-2	2	0	4	48	-4	1.6330	2.2627	-0.4619
3	-2	2	2	0	72	-6	0	3.3941	-0.6928
4	-2	1	-1	5	21	-8	2.0412	0.9899	-9.9238
5	-2	1	1	1	45	-10	0.4082	2.1213	-1.1547

- * The co-ordinates are given in terms of the length $a_0/2$, where a_0 is the lattice parameter of the standard non-primitive unit cell. The co-ordinates relative to O X Y Z are given both in exact form and also numerically to four significant figures. The axes OX and OY are indicated in fig. 3 and OZ is the unit normal to the $(75\bar{1})$.

FIGURE CAPTIONS

- Fig. 1: (a) A partial 200 stereographic projection showing the location of depleted zones A, B and C; depleted zone A is the (220) vacancy platelet.
 (b) A schematic cross-sectional view of the FIM tip which contained depleted zones A, B and C; the plane of projection is the (020) plane. This figure is drawn to scale.
- Fig. 2: A photograph of a ball model of the $(75\bar{1})$ plane built on a (200) plane. The dark balls indicate atoms which are in the outermost (zeroth) layer; the visible atoms within one primitive unit cell, from different layers, are indicated by the numbers 1, 2, 3, 4 and 5. The balls marked with an x indicate one $(11\bar{1})$ plane that intersects the $(75\bar{1})$ plane.
- Fig. 3: The primitive mesh (OABC) of the $(75\bar{1})$ plane and the projection of the atoms that lie within this primitive mesh for planes 1 to 5.
- Fig. 4: A drawing of the atom positions in the zeroth and first layers of the $(75\bar{1})$ plane. The figure is used to explain how the (220) vacancy platelet was reconstructed from the FIM image; see §4 for the details.
- Fig. 5: A series of ten FIM micrographs out of 898 recorded during the atom-by-atom dissection of the (220) vacancy platelet. The solid black dots indicate normal lattice atoms and the open circles indicate vacant lattice sites.
- Fig. 6: The projection of all the vacant lattice sites contained within the (220) vacancy platelet projected onto a (220) plane.
- Fig. 7: An isometric drawing of the (220) vacancy platelet constructed from the maps shown in Fig. 8.
- Fig. 8: Projections of the vacant lattice sites onto the $(0\bar{2}0)$, (200) and (002) planes in Figs. 8a, 8b and 8c respectively. Fig. 8d is a photograph of a ball model taken along approximately a $[\bar{1}00]$ direction; each ball represents a vacant lattice site.
- Fig. 9: A computer generated stereographic pair of the (220) vacancy platelet. Each open circle represents a vacant lattice site and the bond length connecting any two vacant lattice sites is equal to the first nearest neighbor distance ($a_0/\sqrt{2}$). The viewing direction is approximately along an $[0\bar{1}\bar{1}]$ direction.

FIG. 1

FIG. 2

FIG. 3

FIG. 4

FIG. 5

FIG. 6

FIG. 7

FIG. 8

FIG. 9

MASTER

DIRECT OBSERVATION OF THE VACANCY STRUCTURE OF A (220) PLATELET IN AN
ION-IRRADIATED PLATINUM-4.0 at.% GOLD ALLOY

by

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DIRECT OBSERVATION OF THE VACANCY STRUCTURE OF A (220) PLATELET
IN AN ION-IRRADIATED PLATINUM-4.0 at.% GOLD ALLOY[†]

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ABSTRACT

A detailed field-ion microscope (FIM) study has been made of the vacancy structure of a (220) platelet created by a single 30 keV W^+ ion in a platinum-4.0 at.% gold alloy; the specimen was maintained at 40 K (below substage II_B) during the in-situ irradiation at $\sim 2 \times 10^{-9}$ torr. Prior to the pulsed field-evaporation dissection of the specimen at 40 K it was warmed isochronally to 100 K (above substage II_C). The (220) platelet was found to consist of 31 vacant lattice sites, lying in four (220) planes, and clustered in a disc-shaped region which is ~ 20 Å in diameter. If only first nearest-neighbor lattice sites are considered then the distribution of cluster sizes is as follows: (1) two monovacancies; and (2) one jumbo vacancy cluster containing 29 vacancies. The range of the vacancy concentration within the (220) vacancy platelet is ~ 35 to 44 at.%. Employing the modified Kinchin-Pease equation it was calculated that the displacement efficiency (κ) for this platelet is 0.12. It is suggested that the prismatic dislocation loops lying on {220} type planes, observed by transmission electron microscopy, in ion or fast-neutron irradiated platinum can form as a result of the direct collapse of {220} type vacancy platelets.

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§ INTRODUCTION

The point-defect structure of the primary state of damage of irradiated metals can, at present, only be studied experimentally by the field-ion microscope (FIM) technique. The FIM technique provides us with an exact picture of the arrangement of vacant lattice-sites and self-interstitial atoms (SIAs) within and around a depleted zone created by a single primary knock-on atom (Seidman 1973 and 1976). The present paper represents an extension of our earlier research on the body-centered cubic metal tungsten (Beavan, Scanlan and Seidman 1971, Wilson and Seidman 1973) to a face-centered cubic platinum-4.0 at.% gold alloy. There is earlier qualitative work on depleted zones in fast-neutron irradiated platinum by Attardo and Galligan (1966 and 1967) and Inal and Galligan (1970); the main emphasis in this work was in determining size distributions whereas our emphasis is on the spatial distribution of vacant lattice sites within and around individual depleted zones.

In the research on tungsten we studied the point-defect structure of depleted zones created at both 18 K (Stage I) and 473 K (near the top of Stage II); see Schilling, Sonnenberg and Dibbert (1972) for a discussion of Stage II in the Pt(Au) system. The work presented here describes the vacant lattice-site structure of a depleted zone that had collapsed into a four-layer vacancy platelet on a (220) plane. The (220) vacancy platelet was created in the Pt-4.0 at.% Au alloy by a single 30 keV W^{+} ion at 40 K (below substage II_B); the specimen was subsequently annealed to 100 K (above substage II_C) prior to its examination at 40 K. The (220) vacancy platelet represents an energy state that is intermediate in energy between a three-dimensional compact vacancy cluster and a dislocation loop. The possibility of stable multi-layer vacancy platelets does not seem to have been considered in the theoretical literature on this subject. It is suggested on the basis of our observation of this platelet that prismatic dislocation loops, observed in trans-

mission electron microscopy studies of ion or fast-neutron irradiated Pt, can form directly from the collapse of vacancy platelets on {220} type planes. And that the vacancy supersaturation within a platelet required for collapse into a dislocation loop can be exceedingly large. Finally, we present, for the first time, the application of the OR TEP program (Johnson 1965 and 1970) to provide a stereographic drawing of the vacancy platelet.

§2. EXPERIMENTAL DETAILS

2.1. Specimen chemistry and preparation

The Pt-4.0 at.% Au alloy was prepared at Cornell University and the gold concentration was determined to be 4.0 ± 0.3 at.% by the analytical chemistry laboratory of the Materials Science Center and the U.S. Testing Laboratory (see Table I of Chen and Balluffi 1976). The alloy was drawn into 0.13 mm diameter wire and electropolished in a molten salt solution of NaNO_3 and ~20 % by wt. NaCl, maintained at 350°C , to remove any surface contamination. The wires were next annealed by resistively heating them in air at ~1400 K and then air quenched by rapidly terminating the heating current. Sharply-pointed FIM specimens were prepared by the standard electropolishing-technique (Müller and Tsong 1969) at 3 to 4 Vdc, in the above described molten salt-solution, at 623 K. The procedure consisted of dipping a wire specimen, at regular intervals, into the salt bath to a depth of ~5 mm and rapidly removing it after 0.2 sec. Next the FIM specimen was field-evaporated continuously in the FIM at ~125 K and then pulsed field-evaporated at ~70 K to a final end-form at a background pressure of 1×10^{-4} torr Ne.[†]

[†] All pressures reported in this paper have been converted from gauge to real pressure.

2.2. The irradiation procedure

The specimens were irradiated in-situ in a bakeable ultra-high vacuum FIM which is attached to a Hill-Nelson sputtered-metal ion-source via a three-stage differentially-pumped flight-tube (Scanlan, Styris and Seidman 1971). This arrangement allowed for an in-situ irradiation at $\sim 2 \times 10^{-9}$ torr with a pressure of $(2 \text{ to } 5) \times 10^{-6}$ torr argon measured above the diffusion pump which evacuates the ion source. The alloy was irradiated at 40 K with a magnetically analyzed 30 keV W^+ ion beam to a dose of $\sim 1 \times 10^{13}$ ion cm^{-2} and the flux of ions at the specimen position was $\sim 3 \times 10^{10}$ $cm^{-2} sec^{-1}$; at this value of the flux the time required to form an adsorbed monolayer was greater than the irradiation period. After the 40 K irradiation the specimen was annealed isochronally to 100 K (Wei and Seidman 1977).

The specimen temperature was monitored with a miniature platinum resistance thermometer (PRT) mounted near the tail of the cryostat. For further details regarding temperature measurement, the sputtered-metal ion-source and the irradiation facility see our earlier publications (Seidman and Scanlan 1971, Scanlan et al. 1971, Pétroff and Seidman 1973, and Wilson and Seidman 1975).

2.3. Data recording system and ciné film analyzer

The neon FIM images were observed with the aid of an internal image-intensification system based on a Galileo 76 mm diameter channel electron-multiplier array (Brenner and McKinney 1970) and the FIM images produced in this manner were recorded on 35 mm film with the aid of an Automax ciné-camera equipped with a 1000 ft. film chamber. The recorded and developed ciné film was analyzed with a Vanguard motion analyzer which is equipped with x-y cross-hairs and a position readout (Scanlan et al. 1969); the motion analyzer was interfaced to a Houston Omnigraphic 200 x-y recorder. This latter feature was extremely useful for

reconstructing the point defect structure of the depleted zone discussed in this paper. Each FIM image was recorded after a field-evaporation pulse had been initiated; the pulse height and duration were adjusted so that one atom, on the average, was removed per pulse on the (420) plane.

§3. THE ARRANGEMENT OF ATOMS IN THE $(75\bar{1})$ PLANE

The vacancy platelet (depleted zone A) discussed in this paper was detected in the $(75\bar{1})$ plane of an FIM specimen with a $[100]$ orientation. This plane is located on the $[\bar{1}1\bar{2}]$ zone inbetween the (220) and $(53\bar{1})$ planes (see fig. 1a).[†] The interplanar spacing for the $(75\bar{1})$ plane is $a_0/\sqrt{75}$ ^{*} and there are a series of equally spaced planes between the zeroth plane and the 75th plane.^{**} The atomic arrangement within the $(75\bar{1})$ plane and the stacking of the $(75\bar{1})$ planes is a bit complicated, hence we consider this plane in detail.

The crystallography of the $(75\bar{1})$ plane is not given in Nicholas' atlas (1965), hence we constructed a ball model of a $(75\bar{1})$ plane according to the procedure developed by Moore and Nicholas (1961). A photograph of this ball model, built on a (200) plane, is shown in fig. 2; the dark balls indicate the atoms in the outermost (zeroth) layer. The visible atoms, within the primitive unit cell, from

[†] The Miller indices (hkl) of the physical planes must be of unmixed parity for an fcc lattice. If the Miller indices are of mixed parity it is a simple matter to convert them to unmixed parity.

^{*} The lattice parameter of the fcc cell is denoted by a_0 ; for the Pt-4.0 at.%. Au alloy $a_0 = 3.921$ Å (Pearson 1958).

^{**} The number of planes in an identity period (N_{hkl}) is given by the expression $N_{hkl} = QQ^*(h^2 + k^2 + l^2)/2$ where Q is one if h, k, l are all odd and Q is 2 if h, k, l are of mixed parity; and Q* is one if h + k + l is even, while Q* is 2 if h + k + l is odd. It is important to note that in making this calculation one must use the Miller indices (hkl) before they have been converted into unmixed parity. We also note that the Jaswon and Dove (1955) statement "that the stacking pattern of the primitive cubic (hkl) planes constitutes a congruence modulo $h^2 + k^2 + l^2$ " is not generally correct.