Electrons and Holes in Bismuth

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We have re-examined the data published to date that give information (1) on the carrier density per (electron or hole) ellipsoid and (2) on the total carrier density in bismuth at helium temperatures. We show that, in contradiction to some recent conjectures, the number of electron ellipsoids is *three*; the number of light-hole ellipsoids, *one*. The uncertainty in the analysis allows for the possible existence of heavy holes with a number density no greater than ~15% of the light-hole density, assuming that there are no heavy electrons.

INTRODUCTION

IT has been known for more than twenty-five years[1–3] that the Fermi surface for electrons in bismuth can be quite accurately described by a set of equivalent, eccentric ellipsoids in momentum space that enclose $<10^{-3}$ of the Brillouin zone volume, that one principal axis of each ellipsoid is parallel to a crystal axis of twofold rotational symmetry (the "binary" axis), and that the other two principal axes are canted several degrees from the trigonal and "bisectrix" axes. (These three crystal axes are mutually orthogonal and are the axes to which experimental results are most frequently related.) However, the number of crystallographically equivalent ellipsoids and their location in the Brillouin zone has been a subject of conjecture, particularly during the last several years. Similarly, the Fermi surface for holes is now known[4,5] to have the symmetry of an ellipsoid of revolution about the trigonal axis; there is, however, no general agreement upon whether there are two equivalent hole ellipsoids or just one.

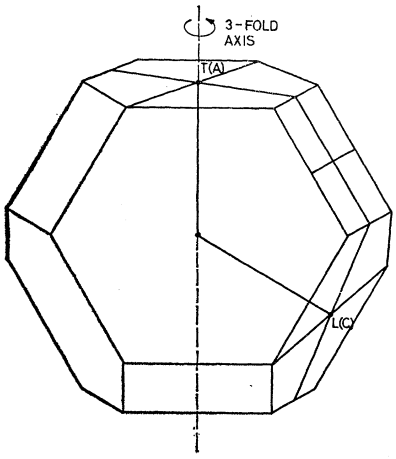

FIG. 1. Brillouin zone for bismuth. Only the two equivalent surfaces with T as their center are regular hexagons. The six other equivalent 6-sided faces with L as their center are "pseudo-hexagonal." The letters in parenthesis are the notation used by Mase (reference 6).

It is the purpose of this paper to point out that from the data in the literature, properly and consistently interpreted, one may demonstrate that there are but three ellipsoids which, judging from the band calculations[6] that do exist, are really six half-ellipsoids centered on the pseudohexagonal faces of the Brillouin zone (points L, Fig. 1). Similarly, there is but one light-hole ellipsoid (and very few if any heavy holes), which presumably is composed of two half-ellipsoids centered on the hexagonal faces of the Brillouin zone[6] (points T, Fig. 1). To show this, one must first consider the experiments that give a value for n (or p), the electron (or hole) concentration per ellipsoid, and then consider the experiments that give N (or P), the total number of electrons (or holes). The first of these include the different experiments that measure the oscillatory behavior[7] of some experimental parameter as a function of the magnetic field H; the de Haas-van Alphen (dH-vA) effect,[1] the magnetothermal oscillations of Kunzler, Boyle, and Hsu,[8] the transport oscillations observed by Steele and Babiskin,[9] and by Connell and Marcus.[10] The period of these oscillations (in H^{-1}) yields directly the cross-sectional area of the Fermi surface, *per ellipsoid*, normal to the magnetic field direction[7]; if the area is measured for a wide enough range of geometries, the volume in momentum space enclosed by the Fermi surface, and thereby n (or p), may readily be computed. Measurements of cyclotron resonance for various orientations, combined with a knowledge of the Fermi energy (obtained, for example, from optical absorption) and either the *assumption of a parabolic band or a theory that gives the momentum dependence of the energy*, also yields a value for the carrier density *per ellipsoid*.

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[2] M. Blackman, Proc. Roy. Soc. (London) **A166**, 1 (1938).

[3] H. Jones, Proc. Roy. Soc. (London) **A147**, 396 (1934); **A155**, 653 (1936).

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[5] J. K. Galt, W. A. Yager, F. R. Merritt, B. B. Cetlin, and A. D. Brailsford, Phys. Rev. **114**, 1396 (1959).

[6] S. Mase, J. Phys. Soc. Japan **13**, 434 (1958); **14**, 584 (1959); W. Harrison, J. Phys. Chem. Solids **17**, 171 (1960).

[7] For a recent review, cf. A. H. Kahn and H. P. R. Frederikse, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1959).

[8] J. E. Kunzler and F. S. L. Hsu, *Proceedings of the Fermi Surface Conference, 1960* (John Wiley & Sons, Inc., New York, 1960), p. 88; J. E. Kunzler and W. S. Boyle, Bull. Am. Phys. Soc. **4**, 168 (1959).

[9] J. Babiskin, Phys. Rev. **107**, 981 (1957).

[10] R. A. Connell and S. A. Marcus, Phys. Rev. **107**, 940 (1957).

There are at least three types of measurements that give values either for N (or P), or what is equivalent for the present purpose, of the *total* area of the Fermi surface: the anomalous skin effect (ASE), the Hall tensor, and the "dielectric plasma anomaly" in optical measurements.[11] Unfortunately, there are two sets of measurements of the ASE in the literature[12,13] that disagree with each other. All other *data* in the literature (as distinct from some published interpretations of that data) relating to n (or p) and N (or P) are mutually consistent. Though one set of ASE measurements[13] is consistent with three electron ellipsoids, we shall disregard the ASE data to avoid controversy.

ELECTRONS

(a) Discussion

There has been a variety of values for n (measured in the liquid-helium region) quoted in the literature which, with the exception of the pioneering work of Shoenberg,[1] fall within the range $(0.8-1.4)\times10^{17}$ electrons per cm^3 per ellipsoid. We believe, as will be shown below, that the best value that may be derived from existing published data is $n=1.4\times10^{17}/\text{cm}^3\pm10\%$. The Hall effect,[14] measured at low temperature, yields $N\lesssim4.1\times10^{17}/\text{cm}^3$. However, the best data for N, the infrared measurements of Boyle and Brailsford[15] (BB) *corrected for the apparently arbitrary ignoration of holes*, yields $N=3.9\times10^{17}/\text{cm}^3$. Therefore the ratio N/n is very close to 3 and shows that there are 3, rather than 6, electron ellipsoids.

The oscillatory experiments, of which the susceptibility measurements are the most complete, unfortunately do not give sufficient information to enable one to obtain the Fermi volume accurately. The largest area (the shortest period), corresponding to the magnetic field along a binary direction, has not been experimentally observed. [A fairly short period observed in magnetoresistance (0.30×10^{-5} G^{-1}) by Babiskin[9] and said to agree with a period that he inferred from Shoenberg's data[1] is in all probability due to holes.[16] The agreement with the dH-vA period for holes[17] is within 30%; the disagreement with the period which we compute below as appropriate is a factor of 3.] The cyclotron resonance experiments, while they can in principle resolve this period, have so far only been reported[5,13,18,19] for geometries in which the magnetic field was along either the binary (1), bisectrix (2), or trigonal (3) direction. Since two of the principal axes of the Fermi ellipsoid are tilted somewhat[1] ($\sim5°$) from the (2) and (3) directions, there are four nonzero tensor mass components in the traditional (1)(2)(3) representation; cyclotron resonance to date has only yielded the values of three in terms of a fourth. However, the optical data of BB, once again corrected for the ignoration of holes, gives an additional independent relation between two of the tensor components.

The "program" we adopt is as follows: From the "classical" cyclotron data of Galt *et al.*[5] and the infrared data of BB,[11] the electron masses are obtained. These are then used with the Fermi energy of 0.022 eV and an energy gap of 0.046 eV (obtained by Weiner[20] from dH-vA measurements on Bi-Te alloys, by Brown *et al.*[21] from an infrared magnetoreflection experiment, and by Wolff,[22] theoretically, from indirect optical absorption) and the recent "nonparabolic, nonellipsoidal" theory of Cohen[23] to calculate the volume enclosed by one "ellipsoid" and thereby a value for n. Using the same theory, and the cyclotron data, de Haas-van Alphen periods are calculated and compared with the best experimental periods, to show consistency of the procedure. The agreement is "perfect." It should be pointed out, as shown very carefully in the work of Weiner,[20] that the masses are highly nonparabolic in the low-mass directions (these masses at the Fermi level are about twice their value at the band edge) and that, therefore, one cannot obtain the Fermi energy by simply multiplying the dH-vA period by the mass obtained either from cyclotron resonance or from the temperature damping of the dH-vA oscillations; this practice, traditional in the literature, has contributed significantly to the confusion that currently exists. Weiner[20] has also shown that the deviations from ellipticity, however, are small. The cyclotron masses of Galt[5] are used here for the reason that, though the Azbel-Kaner resonance masses observed by Aubrey[13,18] are in some disagreement with these, the latest Azbel-Kaner masses measured by Kao[19,24] agree completely with Galt *et al.*[5] The value of n so obtained is then compared with N to obtain the number of ellipsoids.

(b) The Value for n

Boyle and Brailsford[14] have measured the far infrared reflectivity and transmissivity of bismuth as a function

[11] W. S. Boyle, A. D. Brailsford, and J. K. Galt, Phys. Rev. **109**, 1396 (1958).
[12] G. E. Smith, Phys. Rev. **115**, 1561 (1959).
[13] J. E. Aubrey, J. Phys. Chem. Solids **19**, 321 (1961).
[14] A. N. Friedman and S. H. Koenig, IBM J. Research Develop. **4**, 158 (1960), cf. Fig. 3. The magnetic fields used in this experiment were <1.5 Oe, corresponding to $(\mu H/c)\lesssim0.3$ for the highest mobility component.
[15] W. S. Boyle and A. D. Brailsford, Phys. Rev. **120**, 1943 (1960).
[16] The longer period observed by Babiskin is also most probably due to holes, as was pointed out originally by J. E. Aubrey and R. G. Chambers, J. Phys. Chem. Solids **3**, 128 (1957).
[17] N. B. Brandt, A. E. Dubrovskaya, and G. A. Kytin, Soviet Phys.—JETP **10**, 405 (1960); N. B. Brandt, Soviet Phys. **11**, 975 (1960).
[18] J. E. Aubrey and R. G. Chambers, J. Phys. Chem. Solids **3**, 128 (1957).
[19] Y. H. Kao, J. I. Budnick, and S. H. Koenig, Bull. Am. Phys. Soc. **6**, 439 (1961).
[20] D. Weiner, Phys. Rev. **125**, 1226 (1962).
[21] R. N. Brown, J. G. Mavroides, M. S. Dresselhaus, and B. Lax, Phys. Rev. Letters **5**, 243 (1960).
[22] P. A. Wolff (to be published), quoted in reference 19. above.
[23] M. H. Cohen, Phys. Rev. **121**, 387 (1961).
[24] Y. H. Kao (private communication).

TABLE I. De Haas-van Alphen effect periods in units of 10^{-5} G^{-1}. Periods in the second column are computed using Cohen's[a] "nonparabolic nonellipsoidal theory," while in the third column are given the periods recently observed by Weiner.[b] 1′, 2′, and 3′ refer to the principal axes of the ellipsoid.

Direction of H	Calc. period	Observed period
$H\|\|2'$	7.7	8.1
$H\|\|3'$	0.97	0.9
$H\|\|1'$	0.96	(not observed)

[a] Reference 23.
[b] Reference 20.

of frequency for various relative orientations of the crystallographic axis and the infrared polarization. They obtain, experimentally, a dimensionless number, the ratio of two "dielectric plasma anomalies,"[11] which in their notation is given by

$$(\omega_{11}/\omega_{\perp})^2=1.37=2(\alpha_3+\beta_3)/(\alpha_1+\alpha_2+2\beta_1). \quad (1)$$

Here α_1, α_2, α_3 are the diagonal elements of the electron reciprocal effective-mass tensor defined such that $\alpha_i=\partial E/p_i\partial p_i$, and not given by the curvature of the $E-\mathbf{p}$ curve as is normally the case. β_1, β_3 are the corresponding elements for the holes (in this case, the two independent eigenvalues). BB have left out the β terms in Eq. (1) above; doing so gives their Eq. (3). However, Eq. (1) may be immediately derived from Eq. 43 in the appendix of their article. The β's have been measured by cyclotron resonance.[5,19] The values are $\beta_1=14.7$, $\beta_3=1.09$. It is clear that β_1 cannot be ignored in Eq. (1) since $\alpha_1\sim100$, $\alpha_2\sim1$. Substituting the values for β_1, β_3 in Eq. (1) yields

$$\alpha_1+\alpha_2=1.46\alpha_3-27.8. \quad (2)$$

We can now combine these results with the cyclotron data. It must be pointed out here that although the cyclotron resonance determines the masses given by the derivative of the area of the Fermi surface normal to the magnetic field with respect to the energy, one can still use the α's as defined above even in the case of a nonellipsoid nonparabolic theory of the Fermi surface as proposed by Cohen[23] without introducing an error of more than 4% for the case of bismuth. Combining Eq. (2) with the cyclotron data[5] then yields for the reciprocal effective-mass tensor components at the Fermi surface

$$\alpha_1=119, \quad \alpha_2=1.31, \quad \alpha_3=102, \quad \alpha_4=8.6, \quad (3)$$

and for the eigenvalues:

$$\alpha_1'=119, \quad \alpha_2'=2.05, \quad \alpha_3'=101. \quad (4)$$

The above results, together with the Fermi energy and the energy gap, may be substituted into an equation readily derived from Eq. (26), Case A, of Cohen[23] to obtain values for the masses at the band edge; from these values, the values of all pertinent quantities at the Fermi surface may be computed.[25] The value for n, so obtained, is

$$n=1.4\times10^{17}/\text{cm}^3. \quad (5)$$

Values computed for the dH-vA periods are compared in Table I with the observed values; the agreement is proof of the internal consistency of the entire procedure.

(c) Values for N

Bismuth, with one threefold axis, has two independent Hall constants: R_{11}, measurable when H is parallel to the trigonal direction, and $R_{\perp}$, measurable when H is perpendicular to (3). It has been known for some time[4] that R_{11} is positive and very small, whereas $R_{\perp}$ is negative and large. The expressions for $R_{\perp}$, R_{11} in terms of N, P and the respective mobility tensors $\mathfrak{y}$, $\mathfrak{v}$ are [cf. Abeles and Meiboom,[4] Eq. (14)]

$$\begin{aligned}R_{11}&=[N\mu_1\mu_2-P\nu_1^2]/[(N/2)(\mu_1+\mu_2)+P\nu_1^2]^2ec,\\ R_{\perp}&=[(N/2)(\mu_1+\mu_2)\mu_3-P\nu_1\nu_3]/\\ &\qquad[(N/2)(\mu_1+\mu_2)+P\nu][N\mu_3+P\nu_3]ec.\end{aligned} \quad (6)$$

The subscripts here correspond to the components of the mobility tensors along the respective directions. It should be emphasized that the validity of Eq. (6) does not depend on a parabolic dispersion law for the energy; however, the small tilt ($\sim5.5°$) is ignored.

Since $R_{11}\simeq0$, and the mobility anisotropy is similar to the mass anisotropy,[4]

$$\begin{aligned}&N\mu_1\mu_2\simeq P\nu_1^2,\\ &R_{\perp}\simeq[(\mu_1+\mu_2)\mu_3-(2\mu_1\mu_2\nu_3)/\nu_1]/\\ &\qquad(Nec)[\mu_1+\mu_2+2\mu_1\mu_2/\nu_1](\mu_3+\nu_3)\\ &\qquad\simeq(Nec)^{-1}[1+2\mu_2/\nu_1]^{-1}\lesssim(Nec)^{-1}.\end{aligned} \quad (7)$$

The only published data for $R_{\perp}$, taken at low temperatures and at magnetic fields sufficiently low so that the Hall effect is linear in H,[14] give

$$R_{\perp}=15 \text{ cm}^3/\text{C}. \quad (8)$$

Combining this figure with Eq. (7), one obtains

$$N\leq4.1\times10^{17} \text{ cm}^{-3}. \quad (9)$$

A second, more accurate value for N may be obtained from the reflectivity vs frequency data of BB.[15] By fitting the classical expression for the frequency-dependent optical reflectivity of a conductor to their experimental results, BB were able to obtain a value both for the lattice dielectric constant of bismuth (99.6) and for the quantity

$$\omega_0^2=4\pi Ne^2(\alpha_1+\alpha_2+2\beta_1)/2m_0=(162.2 \text{ cm}^{-1})^2. \quad (10)$$

Once again, the term $2\beta_1$ was left out of their analysis.

[25] Equation (26) of Cohen[23] gives the energy-momentum dispersion relation in the neighborhood of the band edge. From this the area, and then the energy derivative of the area, at the Fermi surface may be computed; this latter quantity is the appropriate cyclotron mass. These procedures have been carried through in detail by Weiner[20] and will not be repeated here.

[Physically, including $2\beta_1$ takes into account the fact that the motion of an electron against the background of positive charge can be simply described only in the center-of-mass coordinate system of the electrons and holes; therefore, the reduced mass $m_0/(\alpha_1+\alpha_2+2\beta_1)$ enters into Eq. (10).] From Eq. (10), and the cyclotron mass data, one obtains

$$N=3.9\times10^{17}\ \text{cm}^{-3}. \tag{11}$$

Combining the results in Eqs. (9) and (11) with Eq. (5), one has

$$(N/n)=3.9/1.4=2.8\pm10\% \tag{12}$$

ellipsoids in the conduction band. The $\pm10\%$ is a reasonable estimate of the combined errors in the procedure; i.e., in the cyclotron masses, the Fermi energy, the ignoration of the small ($\sim5\%$) non-ellipsoidal shape of the Fermi surface in the large area cross section,[20,22] etc.

HOLES

(a) Discussion

The situation for holes ought to be, in principle, simpler and more straightforward than for electrons. The symmetry of the hole Fermi surface is higher than that of electrons; also, a set of principal axes of the mass tensor coincides with the (1), (2), and (3) directions. Moreover, the dH-vA measurements of Brandt and collaborators,[17] in which the oscillations due to holes were finally observed several decades after the electron periods were initially seen, at first sight appear to give all the information needed to calculate the Fermi volume exactly. However, careful analysis shows that the data presented (only to be found in the first reference of reference 17) as a function of the angle between the magnetic field and the trigonal direction cannot be fit by an ellipsoidal Fermi surface; the maximum error is $\sim60\%$ if an ellipsoidal surface is assumed and made to agree with the two extremal values. The second paper by Brandt *et al.*,[17] from which the inference may be drawn that the early data have been re-examined, gives values only for the area of the extremal cross sections. The ratio of these areas is equal to the ratio of the cyclotron masses of Galt *et al.*[5] The Azbel-Kaner cyclotron resonance for holes has been observed for holes by Kao[19,24] as a function of the angle of the magnetic field with respect to the trigonal direction. These data, in contrast to the dH-vA data,[17] are fit by an ellipsoidal surface within the experimental uncertainty ($<5\%$); the extremal masses, in addition, agree with those of Galt. In view of this, we choose to believe the Fermi surface ellipsoidal. From the extremal areas as Brandt *et al.*, one obtains

$$P=3.4\times10^{17}/\text{cm}^3=0.87N. \tag{13}$$

Thus, the number of holes *per ellipsoid* is within 15% of the *total* electron concentration. Since no author has as yet proposed, and no data suggest, that $P>N$, there can be but one hole ellipsoid. There has been the suggestion made[17,26–28] from time to time that a third set of carriers, heavy holes, may exist. The analysis above allows for a total concentration of these carriers of only $5\times10^{16}/\text{cm}^3$ (unless heavy electrons also exist); this number could equally well be zero within the uncertainty of the analysis.

It should be pointed out that in a recent review article, Boyle and Smith[29] essentially use an ellipsoidal model for the hole Fermi surface to fit Brandt's data at but one point, this point being where the difference from the fit that we have used is maximum. The 60% mentioned above becomes a factor of 2 ($1.6^{\frac{3}{2}}=2.02$) when p is computed. We feel that, because of the agreement of the extremal values of Brandt with the cyclotron data and the good fit of Kao's cyclotron data to an ellipsoidal surface, our choice of the dH-vA data is correct. Moreover, since the masses of the holes are much greater than those of the electrons (holes in bismuth are much like electrons in germanium), the valence band should be parabolic in all directions, at least to the hole Fermi energy ($\sim10^{-2}$ eV), if only by analogy with the conduction band of germanium. In the parabolic case, the dH-vA areas and the cyclotron masses (related to the energy derivative of the area) should be strictly proportional; for our choice of the dH-vA data, they are.

GENERAL REMARKS

To recapitulate, there are three electron "ellipsoids" in bismuth with a density of 1.4×10^{17} electron per cm^3 per ellipsoid. The data for holes, as we have chosen to interpret them, give a light hole density per ellipsoid very close to that of the *total* electron density N. Were the hole data to be interpreted in the other extreme,[29] the value for the hole density per ellipsoid becomes *twice* N; among all the models proposed for the conduction and valence bands of bismuth, no one has suggested this possibility.

The best value for the Fermi level for holes, consistent with the preceding remarks, calculated using the cyclotron masses and the dH-vA areas, is 12×10^{-3} eV.

It is also clear that with all the oscillatory data that have been obtained for bismuth to date, there is still a need for a definitive set of measurements as a function of orientation to be made.

A remark must be made concerning Weiner's[20] paper. He has studied the dH-vA effect in bismuth doped with tellurium and has shown quite clearly that Cohen's[23] model, with electron ellipsoids at points L, Fig. 1,

[26] V. Heine, Proc. Phys. Soc. (London) **A69**, 513 (1956).
[27] I. N. Kalinkina and P. G. Strekov, Soviet Phys.—JETP **7**, 426 (1958).
[28] J. R. Sybert, C. G. Grenier, and J. M. Reynolds, Bull. Am. Phys. Soc. **7**, 74 (1962).
[29] W. S. Boyle and G. E. Smith (review article to be published).

describes the nonparabolicity very well. None of this requires any statement about the number of electrons donated per Te atom. Weiner then makes the *assumption* that one Te atom donates one electron, and from this concludes that there are six electron ellipsoids. The point we wish to make is that there is no basis for this assumption. For example, it is known[30] that Sn, which along with Te is one row above Bi in the periodic system, produces three times the change in hole concentration that Pb does. (Pb is immediately to the left of Bi in the periodic system.) Then, the recent work of Brandt and Razumenko[31] shows that Pb only reduces the *electron* concentration by one electron per ellipsoid per 55 Pb atoms added. Moreover, if one just thinks a bit about what $\sim 10^{-2}\%$ Te in Bi does, one realizes that the "impurity band" width may well be of the order of the electron Fermi energy.[32] All this means that, at the least, it would be more prudent to use the existence of three ellipsoids to show that each two Te atoms add approximately one electron than to argue the other way.

[30] V. Heine, Proc. Phys. Soc. (London) **A69**, 505 (1956).
[31] N. B. Brandt and M. V. Razumenko, Soviet Phys.—JETP **12**, 198 (1961).

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[32] Experiments on heavily doped germanium indicate that the band structure is not perturbed by large concentrations of impurities [cf. M. Pollak, Phys. Rev. **111**, 798 (1958)]. Presumably the situation is similar in bismuth, as Weiner's work suggests.

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Point Defects in Copper*‡

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The atomic configurations and energies for point defects in copper have been studied theoretically using a classical model. The atoms near the defect are treated explicitly while the remainder of the crystal is treated as an elastic continuum with atoms imbedded in it. A Born-Mayer repulsive force law, Ae^{-ar}, is assumed to act between nearest neighbors. Vacancies, interstitials, di-vacancies, and di-interstitials have been considered. Configurations are found by choosing a starting configuration roughly approximating the situation under consideration, and an iterative process of successively adjusting the value of each variable occurring in the equation for energy such that the magnitude of the generalized force acting on it is minimized. The energy calculations include changes in bond energy in the discrete region, energy in the elastic field, and work done against cohesive forces, but neglect changes due to the redistribution of electrons. Various aspects of the model and method of calculation have been investigated, and the effects of electron redistribution are discussed. Predicted activation energies for motion of interstitials and vacancies are 0.05 and 0.43 eV, respectively. An upper limit of 0.26 eV has been found for the activation energy for migration of di-interstitials. The isolated interstitial has been thoroughly investigated, and eight well-defined equilibrium configurations have been found. Only one of these is stable, being the case in which two atoms are symmetrically split in the ⟨100⟩ direction about a vacant normal lattice site. The configuration in which the interstitial is located at a body center is found to be a local maximum, but the saddle point configuration for migration of interstitials is quite close to it.

INTRODUCTION

THE determination of atomic configurations and energies associated with point defects in metals has been the subject of a number of calculations.[1–11] The primary interest is in activation energies for motion and the associated atomic mechanisms. Therefore, metastable and saddle-point configurations must be investigated as well as the stable configuration. To a good approximation, the configurations may be determined by regarding the atomic coordinates classically (i.e., neglecting zero-point motions), but subject to forces which have essentially quantum mechanical

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