ed by the higher minima than that on tellurium suggests that sulfur and oxygen will provide defects where the simple hydrogenic model for Γ_1 minima is even less applicable.

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STACKING-FAULT ENERGY AND MANY-BODY FORCE EFFECTS IN SOLID ARGON

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A stacking fault in fcc solid argon is an interesting defect because a fault converts a region of the crystal into the hcp structure. The energy per unit area, γ, required to create this defect is then a measure of the binding energy increase, δU, of solid argon when condensed in the hcp rather than the fcc phase. Determining this difference, δU, has been a problem of long standing interest[1] because the two-body potentials of the Mie-Lennard-Jones type, used extensively, all predict a lower binding energy for the hcp structure[2] (δU negative), whereas fcc argon is observed naturally. This theoretical error is thought to arise from approximating the many-body interactions by a sum of two-body interactions[2] between individual atoms.

An experimental measurement of γ can be used to determine the real difference, δU, if the relative values of γ and δU are known. For this reason, the stacking-fault energy of argon has been calculated for the case when the crystal atoms interact through a two-body Lennard-Jones (6, 12) potential,[3]

$$V(R) = \epsilon[r_0/R)^{12} - 2(r_0/R)^6],$$

with $\epsilon = 164.3 \times 10^{-16}$ erg and $r_0 = 3.818$ Å, which is known to favor hcp by $\delta U = -0.01\%$,[2] giving $\gamma = -0.022$ erg/cm^2. To get this accurate estimate of γ, it was found necessary to include over 240 shells of atoms in each spherical volume that intersects the fault plane. A similar calculation[4] using the three-body forces of Jansen and Zimmering,[5] which favors fcc argon by $\delta U/U \simeq 6\%$, gives $\gamma = 10$ erg/cm^2.[6] Using these results and the origin we can obtain an approximate (nearly linear) relation between γ and $\delta U/U$. This linear relationship is eqivalent to saying that a stacking fault is a region of hcp which is 1.9 (111) planes thick in all the rare-gas solids.

Figure 1 shows an election micrograph of

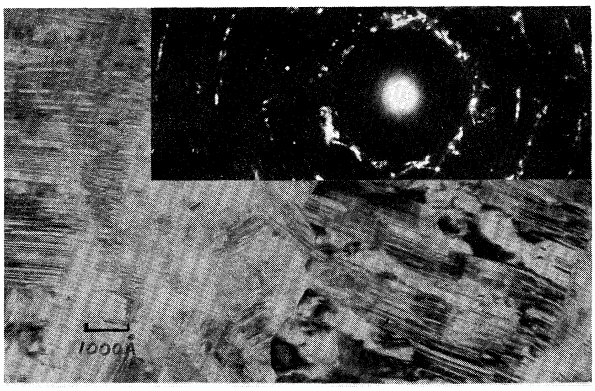

FIG. 1. Electron micrograph and diffraction pattern of solid xenon.

solid xenon and its associated diffraction pattern.[7] The xenon film was grown on a carbon substrate at as high a temperature as was possible in the microscope vacuum to increase the grain size, namely about 60°K, and photographed below 20°K. The main point to notice is that each grain contains a high density of parallel lines which are stacking faults, twins or regions of hexagonal phase. The diffraction pattern bears this out with its long streaks and spots at positions intermediate for those of the fcc and hcp structures.

From inspection of this picture (and similar ones of solid argon[7]) it seems certain that the fault energy, γ, for the rare-gas solids must be lower than that for fcc metals such as Ag, which show no such comparable density of faults in evaporated films. By lower we clearly do not mean just $\gamma_{Ar} < \gamma_{Ar}$, since the binding energies of the two solids are so different. In comparing γ_{Ar} and γ_{Ag} numerically we must correct for the difference in absolute binding energy per unit area of the two solids. Experimentally U is approximately proportional to μa_0, where a_0 is the nearest-neighbor spacing and μ the shear modulus, for all the rare gases and for silver. Thus the observation of a greater fault density in argon than in silver means $(\gamma/\mu)_{Ar} < (\gamma/\mu)_{Ag}$.

Using the best values of $\gamma_{Ag} \sim 20$ erg/cm^2,[8] the above approximate argument leads to $\gamma_{Ar} \lesssim 0.7$ erg/cm^2 and $\gamma_{Xe} \lesssim 1.0$ erg/cm^2. These values, using the approximately linear relation between γ and δU, mean that $\delta U/U$ for solid argon is $\lesssim 0.4\%$, which is $\simeq 1/15$th that predicted by the calculations of Jansen and Zimmering.[5] This means that many-body effects, although important for the particular problem of stability, contribute very little to the total binding ($\lesssim 0.4\%$) in rare-gas crystals. For practical purposes the two-body force picture is a very adequate one.

Further work is now being undertaken by one of us (JAV) to measure γ more accurately by observation of individual dislocations in these condensed films.

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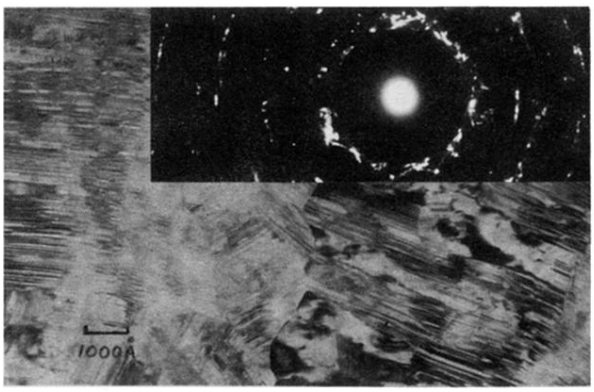

FIG. 1. Electron micrograph and diffraction pattern of solid xenon.