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Embedded-atom-method study of coherency and elastic moduli of Pd-Cu multilayers

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The embedded-atom method was utilized to study coherent and incoherent interfaces and elastic moduli in Pd-Cu multilayers with wavelengths of 2, 4, and 6 monolayers (ML) of (111) planes. The multilayer with a wavelength of 2 ML was coherent, and the multilayer with a wavelength of 6 ML was incoherent with a misfit dislocation structure similar to a Pd-Cu bicrystal. The lattice of the multilayer with wavelength of 2 ML was highly strained with a lattice parameter of 3.83 Å within the (111) plane and a lattice parameter of 3.66 Å normal to the (111) planes. In the incoherent multilayer the lattice parameter normal to the (111) planes was larger than the coherent multilayer, but the total volume of the incoherent multilayer was less than the coherent multilayer, indicating that atoms had relaxed into lower-energy positions with the formation of misfit dislocations. Elastic moduli that related stresses to strains where the registry of the (111) planes was not distorted were observed to increase as the volume (or coherency) decreased. Elastic moduli that related stresses to strains that distorted the registry of the (111) planes were observed to increase as coherency (or volume) increased. Changes in moduli calculated were typically 10–20 %.

INTRODUCTION

Multilayer materials are of significant interest because through layering of the materials it is possible to obtain physical properties that are unique to the layering periodicity. Examples of this are changes in the electronic band structure in strained quantum-well field-effect transistors[1] and the development of x-ray reflectors with unique periodicities.[2] Another property that depends upon the layering periodicity is the "supermodulus" effect that has been observed in several multilayers including Pd-Cu.[3] The "supermodulus" effect is the 100–300 % increase in elastic modulus that has been reported at particular wavelengths in multilayers. Typical behavior reported for large wavelengths is that the elastic moduli obey the standard equations for the isostrain or isostress model of composite materials. However, for wavelengths from 20 to 30 Å, such as in the Ag-Pd system, a 300% increase in elastic modulus has been reported.[4] At smaller wavelengths the supermodulus effect disappeared; this disappearance of the supermodulus effect may be a result of the experimental inability to produce separate layers at thicknesses that approach 1 monolayer (ML). In another example, Hilliard and co-authors[3] reported a biaxial modulus more than 3 times that expected from a simple mixture of the atoms for a multilayer of (111) planes of Pd and Cu with a wavelength of 14.7 Å.

There are several theories that have been proposed to explain the supermodulus effect. One theory proposes that the supermodulus effect is due to coherency strains that result when the two crystals of different lattice parameter are each strained, one in compression and one in tension, to a common equal lattice parameter. One recent study of the effect of coherency strain was that of Jankowski.[5] In this work the repulsive ion core interaction was utilized to estimate the elastic moduli as a function of strain. It was found that the biaxial modulus increased as the multilayer was compressed, and it decreased as the multilayer was strained in tension. It was assumed that each layer in the unstressed multilayer had a uniform strain that could be calculated from the misfit and the elastic moduli. The strains in the two lattices were approximately equal and opposite. The total modulus was calculated by taking the average of the individual layer moduli. Calculations of the biaxial modulus

by Jankowski predicted increases of 15 to 50% for systems such as Au-Ni; whereas, experimental increases of over 100% were reported.[3]

Clemens and Eesley[6] have demonstrated that the atomic planes within a layer with multiple monolayers are not uniformly spaced, and that the interplaner spacing for planes at the interface can be greater than for planes away from the interface. Clemens and Eesley developed a model incorporating the "universal equation of state" to relate the interface strain to elastic moduli and explained decreases (softening) of the elastic modulus in systems such as Mo-Ti. Cammarata and Sieradzki[7] developed a thermodynamic model that incorporates decreases in interplanar spacings at an interface to predict increases of approximately 50% in elastic moduli (supermodulus effect) for multilayered thin films. Cammarata and Sieradzki predict the supermodulus effect to occur for incoherent layers and to disappear for coherent layers.

As can be seen from the above discussion, there is considerable disagreement as to the origin of the supermodulus effect and whether it occurs in multilayers that are coherent or incoherent. For these reasons, it is desirable to study the relationship of elastic moduli to coherency with more fundamental models that make as few assumptions as possible and allow for crystal relaxation.

METHOD OF ANALYSIS

In this analysis of multilayered materials the embedded-atom method (EAM) was utilized in conjunction with an energy minimization procedure based upon the conjugate gradient technique.[8] The EAM developed by Daw and Baskes[9] includes a pair potential to account for repulsive interactions and an embedding energy term that includes many-body effects into the total cohesive energy. The local electron density is calculated for the relaxed atomic positions by summing the atomic electron densities for all the surrounding atoms. In previous work, it has been demonstrated that interface relaxations can be calculated with the EAM.[10]

In this study of multilayers Pd and Cu were selected for the study because elasticity calculations predicted that a transition from coherent to incoherent interfaces with misfit dislocations would be observed with layer thickness of only a few monolayers. Embedding functions are available for Pd and Cu from the work of Foiles, Baskes, and Daw.[11] The atom configuration utilized was 4417 atoms in a sphere with a nominal radius of 25 Å. The multilayer had equal numbers of (111) planes of each atom type and layer thicknesses of 1, 2, and 3 ML were utilized resulting in wavelengths of 2, 4, and 6 ML. All atoms were initially placed in positions corresponding to a Pd lattice parameter (3.89 Å). In the energy minimization at 0 K and zero pressure, all atoms were relaxed to minimum energy positions, and no constraints or forces were placed on the surface atoms. The energy minimization was performed with the Dynamic Code Version 5.2 written by Daw and Foiles.[12]

The elastic constants were calculated by starting with the multilayer atoms in their relaxed positions and then straining the lattice in small increments of both positive and negative strain, and calculating the total crystal cohesive energy. Strain increments were always sufficiently small that the energy for positive negative strains were nearly equal.

RESULTS

The results of the energy minimization showed that for a wavelength of 2 ML the Pd and Cu monolayers were coherent, for a wavelength of 4 ML there were regions of coherency and regions where misfit dislocations were starting to form, and for a wavelength of 6 ML misfit dislocations were present in a configuration essentially the same as was calculated for a Pd-Cu bicrystal.[10] These results are shown in Figs. 1 and 2. Figure 1(a) shows the Pd atoms (solid circles) and Cu atoms (open circles) on both sides of a Pd-Cu interface. The Pd and Cu atoms are in perfect registry except for some small displacements at the sphere surface. This conclusion is confirmed by Fig. 2(a), which shows that the lattice parameters are equal within the (111) plane in the $[11\bar{2}]$ direction for both the Pd and the Cu layer. The lattice parameter was calculated from the interatomic distances in the $[11\bar{2}]$ direction (note that at the free surface additional relaxations occur).

Figure 1(b) shows the Pd and Cu atom positions on either side of a Pd-Cu interface in a multilayer with a wavelength of 4 ML. In Fig. 1(b), it appears that much of the interface is coherent with the Pd and Cu atoms in registry; however, at the edges of the sphere in three directions the atoms of one layer are pushed to the saddle point of the other layer due to the misfit strain. This is where the Pd and Cu atoms form lines of atoms in Fig. 1(b). The lattice strain can be also be seen in Fig. 2(b), which shows the lattice parameter within the (111) plane as a function of position in the $[11\bar{2}]$ direction. This direction in Fig. 1(b) corresponds to the vertical direction through the center point. In Fig. 2(b) for negative positrons [bottom of Fig. 1(b)] the lattice was coherent with the Pd and Cu layers having essentially the same lattice parameters. For positive positions significant differences in lattice parameter were calculated; the atoms in the Cu layer were significantly compressed together relative to the Pd atoms. The compression of the Cu lattice and the expansion of the Pd lattice is indicative of lattice strain that is necessary for the formation of a misfit dislocation. The presence of misfit dislocations in the multilayer with a wavelength of 6 ML is more clearly shown in Figs. 1(c) and 2(c). In Fig. 1(c) the straight lines of Pd and Cu atoms indicate where the Pd and Cu atoms are at saddle points relative to each other, and for atoms outside the straight lines the Pd and Cu atoms have been shifted by a partial dislocation Burgers vector of the type $\frac{1}{6}[11\bar{2}]$ relative to each other. This displacement was previously explained in more detail.[10] The lattice strain within the (111) planes can also be seen in Fig. 2(c) for six different layers in the multilayer. Note again that adjacent Pd and Cu layers such as the +1 (Cu) and +2 (Pd) layers have some regions where the lattice parameters are similar and some regions where the Pd and Cu monolayers have

significantly different lattice parameters. The layers +1, +2, etc., refer to the position in layers relative to the zero layer measured in monolayers. Note that there are some regions of the Cu layers with atomic spacings less than the equilibrium Cu lattice parameter and some regions of the Pd layers with atomic spacings greater than the Pd equilibrium values. The atomic displacements observed in Fig. 1(c) were essentially the same as those observed in a bicrystal.[10] Thus for Pd-Cu a wavelength of 2 ML was fully coherent, and a wavelength of 6 ML had a misfit dislocation arrangement essentially the same as a bicrystal. Increasing the wavelength further would not be expected to result in any significant change in the misfit dislocation arrangement at the interface.

The results of the EAM simulation of lattice displacements can be compared to the theory recently proposed by Jesser and van der Merwe (JvdM) that treats multilayer materials of unequal elastic constants with a theory of elasticity stress function approach.[13] The JvdM theory predicts a lattice parameter of 3.76 Å for the coherently strained Pd-Cu lattice. This calculation includes the differences in shear modulus and Poisson's ratio for Pd and Cu; for Pd and Cu the shear moduli utilized were 0.0543 and 0.0593 GPa; the Poisson's ratio utilized were

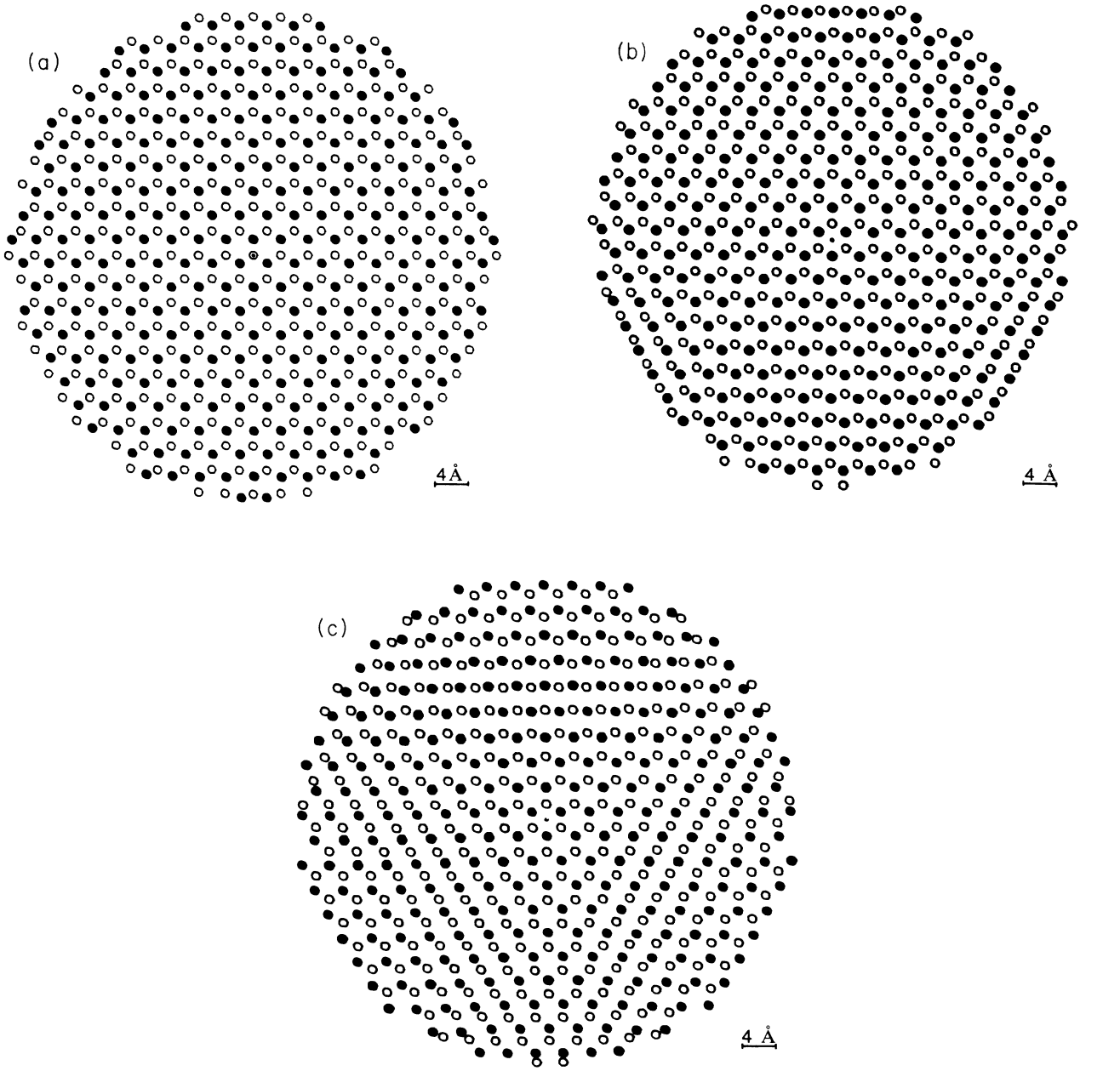

FIG. 1. Top view of Pd atoms (solid circles) and Cu atoms (open circles) for adjacent Pd and Cu (111) planes. X is the position of the planes measured in monolayers (ML). (a) $X(\mathrm{Pd})=+1$ and $X(\mathrm{Cu})=0$ ML for the wavelength of 2 ML. (b) $X(\mathrm{Pd})=+2$ and $X(\mathrm{Cu})=+1$ ML for the wavelength of 4 ML. (c) $X(\mathrm{Pd})=+2$ and $X(\mathrm{Cu})=+1$ ML for the wavelength of 6 ML.

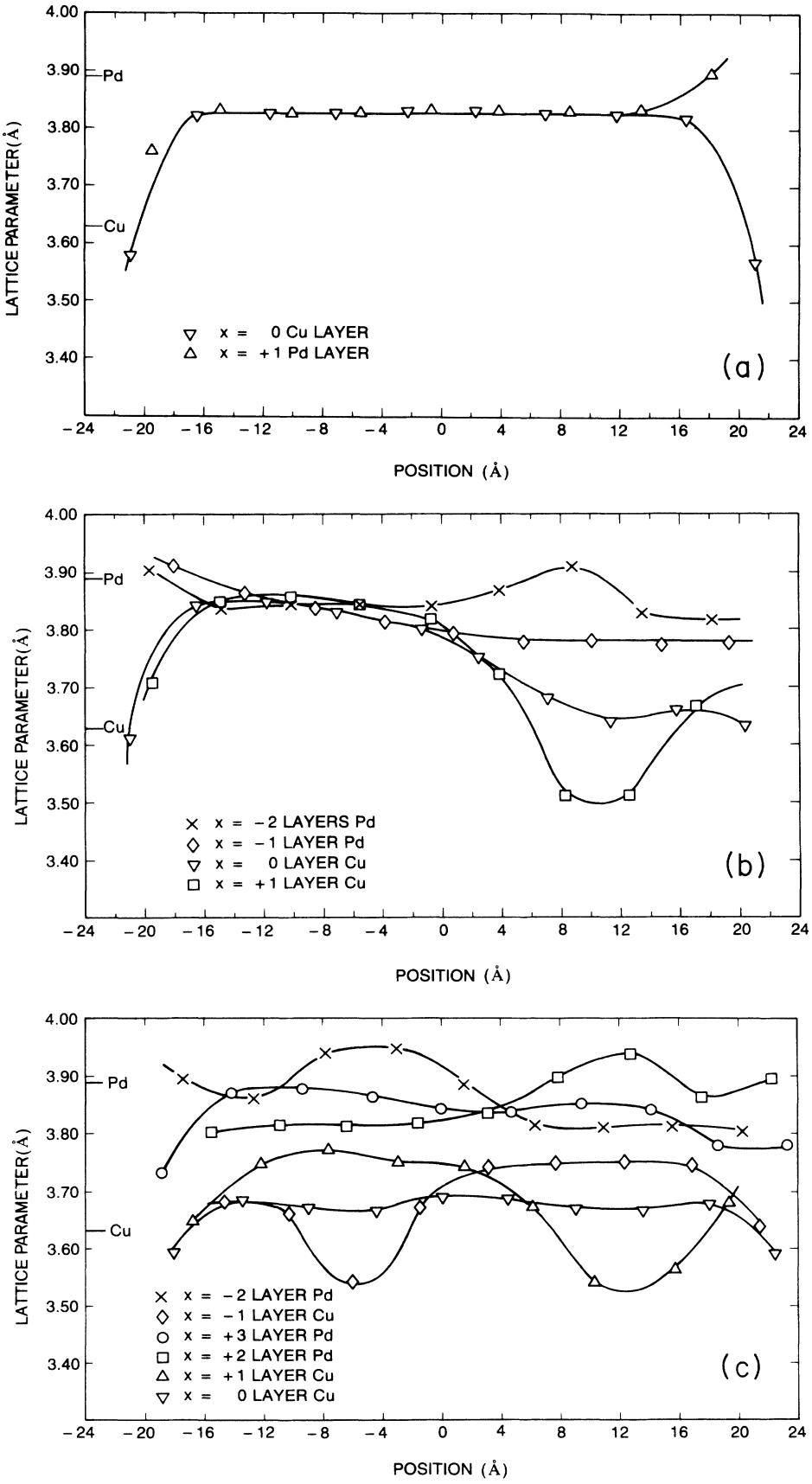

FIG. 2. Lattice parameter within the (111) planes in the $[11\bar{2}]$ direction calculated from the interatomic spacings as a function of position across the sphere model. (a) Wavelength of 2 ML, (b) wavelength of 4 ML, (c) wavelength of 6 ML.

0.373 and 0.317,[14] and the lattice parameters utilized were 3.89 and 3.62 Å. In this calculation, it is important to include the differences in Poisson's ratio because this difference has a greater effect than the elastic modulus difference. The EAM analysis resulted in a lattice parameter of approximately 3.83 Å in the $[11\bar{2}]$ direction for the coherent lattice with the wavelength of 2 ML. The lattice parameter normal to the (111) planes in the same multilayer was 3.66 Å when averaged over six layers. All interplanar spacings normal to the (111) interfaces for the wavelength of 2 ML are between Pd and Cu layers. The spacing normal to the (111) planes for wavelengths of 4 and 6 was 3.75 and 3.74 Å, respectively, when averaged over the same six layers. Because of this change in shape of the sphere, it was necessary to determine an average radius for the sphere from four points, one on the top, one on the bottom, and two points on the equator at opposite sides of the sphere.

The JvdM theory can also be utilized to predict the critical strain that can be accommodated without the formation of misfit dislocations as a function of multilayer thickness. For these Pd-Cu multilayers with equal numbers of Pd and Cu monolayers per layer, the critical misfit is plotted in Fig. 3 as a function of wavelength in terms of the number of monolayers per wavelength, where it was assumed that the thickness of 1 ML was $c/\sqrt{3}$ where $c=3.75$ Å is the reference lattice parameter from equation 2 in JvdM,[13] and interface properties were assumed to be an average of the Pd and Cu properties. Since the misfit in Pd-Cu is 7.2%, the results plotted in Fig. 3 would predict that a multilayer with a wavelength of 2 ML should be coherent. A multilayer with wavelength of 4 ML should have misfit dislocations; however, most of the strain should be accommodated by elastic misfit strain because the total misfit (7.2%) is only slightly more than the critical misfit of (6.8%) and thus approximately 0.4% strain would be accommodated by misfit dislocations. These results for the critical strain are in excellent agreement with what was calculated with the EAM simulations where the multilayer with a wavelength of 2 ML was coherent, and the multilayer with a wavelength of 4 ML showed the initial stages of misfit dislocation formation; and a multilayer with a wavelength of 6 ML had misfit dislocations similar to a bicrystal.

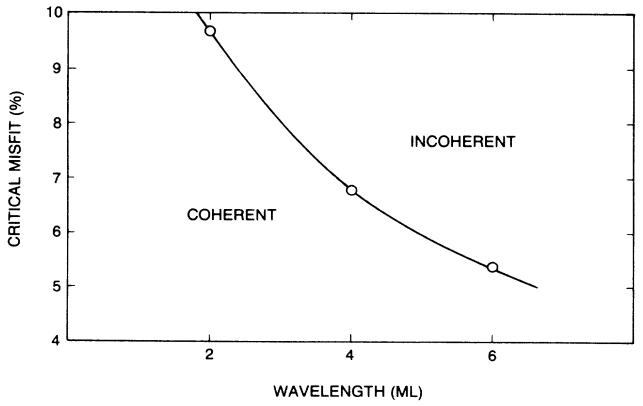

FIG. 3. Critical misfit as a function of wavelength in monolayers based upon the theory of Jesser and van der Merwe (Ref. 13). The misfit for Pd-Cu is 7.2%.

ELASTIC MODULUS RESULTS

To test the EAM calculations of the elastic properties for the chosen configuration, the elastic moduli of Pd were first calculated. The bulk modulus was calculated by straining the sphere in increments of ± 0.0002 along each axis to a maximum of ± 0.002 strain. The total cohesive energies for 4417 atoms were symmetrical to within ± 0.04 eV for strains of ± 0.002; this indicates that the presence of the surface was not having a significant effect on the energies, for surface effects should result in different energies for negative strains relative to positive strains. From the bulk modulus and the constant volume axial modulus, the elastic constants for a cubic isotropic solid C_{11} and C_{12} were found utilizing the equations of Mott and Jones,[15] and C_{44} was determined by imposing a shear deformation. The shear moduli C_{yxyx}, C_{xyxy}, and C_{yzyz} were also determined by imposing shear deformation on the sphere; the directions here are X [111], Y $[1\bar{1}0]$, and Z $[11\bar{2}]$.

The second derivatives of total cohesive energy (E_c) with respect to strain were evaluated at zero strain by fitting the cohesive energy versus strain data to a polynomial; the second derivative was then twice the coefficient of the second-order term. No large differences were observed for the second derivative if a polynomial of second order or fourth order was utilized; this indicates that the stresses were linearly dependent upon the strains obeying Hooke's law. The second-order polynomial was utilized for the data presented in Tables I and II. There is good agreement between experimental results and the EAM calculations for the bulk modulus, C_{11} and C_{12} and C_{44} as shown in Table I. The difference in the shear moduli indicates the anisotropic properties in the Pd crystal. The good agreement between the calculated elastic moduli for the 4417 atom sphere and experimental results for Pd indicates that the chosen configuration of atoms should yield reasonable results for calculated multilayer elastic moduli. The biaxial modulus was calculated by straining the multilayer crystal by an amount ε in the Y and Z directions within the (111) planes and by $-2\nu\varepsilon$ in the X direction, which is perpendicular to the (111) planes. For Pd, $\nu=0.373$, and for Cu, $\nu=0.317$, and thus for the multilayers $\nu=0.345$ was assumed. With this strain the biaxial modulus (Y) was calculated from the equation

TABLE I. Elastic moduli of Pd in GPa.

Modulus	Calculated	Experimental (Ref. 14)
C_{11}	0.222	0.234
C_{12}	0.172	0.176
C_{44}	0.064	0.071
Bulk	0.189	0.196
Biaxial	0.279	
C_{yxyx}	0.033	
C_{yzyz}	0.048	

TABLE II. Calculated elastic properties of multilayers in GPa.

Wavelength (ML)	2	4	6	Pure Pd
Properties				
Atomic volume (Å^3)	12.39	12.23	12.10	14.02
a normal to (111) Å	3.66	3.75	3.74	3.89
Bulk modulus	0.194	0.178	0.172	0.189
Biaxial modulus	0.263	0.274	0.281	0.279
C_{xyxy}	0.040	0.039	0.036	0.032
C_{yxyx}	0.040	0.040	0.037	0.033
C_{yzyz}	0.050	0.052	0.055	0.048

$$Y=\frac{1}{2V}\left[\frac{\partial^2 E_c}{\partial \varepsilon^2}\right]_{\varepsilon=0}. \quad (1)$$

The biaxial modulus of Pd was calculated to be 0.279 GPa, as shown in Table I, and this compares with a value of 0.27 GPa measured by Yang and co-workers[3] for a Pd-Cu multilayer.

The initial atom positions for elastic-moduli determination were the relaxed atomic positions as discussed above. Thus, the multilayer with a wavelength of 6 ML contained misfit dislocations and the multilayer with a wavelength of 2 ML was coherently strained. The results of the elastic constants calculations for the multilayers are shown in Table II.

DISCUSSION

The most obvious result from this study of the elastic constants of multilayered materials is that the changes in elastic moduli were not of the magnitude of some experimental observations.[3,4] However, recent experiments have not been able to reproduce the previously measured supermodulus effects, and this has raised questions about the validity of the initial reports of supermodulus effects. If the supermodulus effect is valid, then the EAM in combination with the modeling procedures incorporated in this work did not result in a large supermodulus. The effects of coherency are included in this study as are the interface strain energy effects, and thus this study indicates that these do not account for the magnitude of a large supermodulus effect.

Although this study did not result in the observation of a large supermodulus, the results relate to the models that have been proposed, and some correlations of moduli and coherency did occur. The coherency models[5,16] are based upon the observation that the elastic moduli increase at a faster rate in compression than they decrease in tension. The EAM study showed that for the coherent multilayer within the (111) planes the Pd lattice was compressed much less (-1.5%) than the Cu lattice was expanded ($+5.5\%$); however, Jankowski and Tsakalakos assumed that strains were nearly equally distributed between tension and compression. Based upon these EAM results this assumption should be reconsidered. Coherency effects were included in the EAM study through the variation of the wavelength, and the biaxial modulus was the smallest for the coherent multilayer; however, other moduli such as the bulk and some of the shear moduli were increased by coherency.

The model of Cammarata and Sieradzki[7] predicts that the biaxial supermodulus effect should disappear for coherent multilayers and should be present in the case of noncoherent interfaces, and this trend was observed in this study; however, the magnitude of the biaxial modulus increase resulting from this study was only 7%. This study should include the effects discussed by Cammarata and Sieradzki such as lattice expansion or contraction normal to the (111) interface and interface strain. The spacing normal to the layering was reported by Clemens and Eesley[6] and by Cammarata and Sieradzki[7] to be related to the elastic moduli; increased spacing resulting in lower moduli and decreased spacing resulting in higher moduli. For a wavelength of 2 ML, where the Pd and Cu lattices were coherent, the interplanar spacing normal to the (111) planes contracted 2.7% relative to the reference lattice parameter of 3.76 Å. The biaxial modulus was a minimum for this multilayer. Wolf and Lutsko[17] reported on an EAM and Lennard-Jones simulation of multilayers of Cu where the Cu layers were rotated relative to each other. An increase in lattice parameter perpendicular to the layers was accompanied by an increased Young's modulus parallel to the layers. These results correlate with the results of this study. However, this increase in modulus may be due to the decrease in volume that was observed, because elastic moduli are inversely related to atomic volume.

Analysis of the results in Table II indicates that the expansion normal to the highly strained planes of a multilayer allows the atoms within the planes more space for relaxation, thus decreasing the volume of the crystal. The relaxation and subsequent volume contraction could explain the increases in biaxial modulus parallel to the (111) planes and the shear modulus within the (111) planes C_{yzyz}. The bulk modulus and the shear moduli C_{xyxy} and C_{yxyx} which relate to shear displacements parallel and perpendicular to the (111) planes, respectively, increase as volume increases, and thus they would appear to be a result of coherency effects. The biaxial deformation and the shear strain γ_{yz} both deform the crystal without any component of the strain tending to disrupt the atomic registry of the (111) planes because all of the (111) planes are deformed by the same strain, whereas the hydrostatic strain and the strains γ_{xy} and γ_{yx} all have components of strain that alter the registry of the atoms in the (111) planes. The hydrostatic strain disturbs the registry because the strains are radial, whereas the struc-

ture is planar. The moduli related to strains that distort the registry of the (111) planes all increased as coherency increased, whereas moduli that relate to strains that did not distort the coherency increased as coherency decreased or as volume decreased.

CONCLUSIONS

(1) The EAM in conjunction with a model of a multilayer with free surfaces was effective in modeling multilayer interfaces. It was observed that a multilayer of 2 ML (1 Pd and 1 Cu) was coherent with a lattice parameter of 3.83 Å parallel to the (111) planes and 3.66 Å perpendicular to the (111) planes in comparison to an average (reference) lattice parameter of 3.75 Å. For a wavelength of 6 ML (3 Pd and 3 Cu) the interface contained misfit dislocations with essentially the same arrangement as appeared in Pd-Cu bicrystals. In the incoherent lattice, the atomic spacings in the $[11\bar{2}]$ direction within (111) planes had regions of compression and tension as would be expected if misfit dislocations were present; and in the direction normal to the (111) planes the lattice relaxed to an average value of 3.74 Å. The atomic volume of the coherent lattice was the highest and the atomic volume of the incoherent lattice was the lowest. The transition from coherent to incoherent interfaces calculated with the EAM was in excellent agreement with the analytic theory of Jesser and van der Merwe[13]; however, lattice parameters calculated with the two approaches differed significantly. This difference is probably due to the nonsymmetric nature of the interatomic potential at high strain (7.2%).

(2) Elastic moduli of Pd and the Pd-Cu multilayers were calculated including bulk, biaxial, and shear, and the results for Pd were in good agreement with published values. No large "supermoduli" were observed. Moduli related to strains that did not distort the registry of the (111) planes were observed to increase when the lattice relaxed, resulting in misfit dislocations and a reduced volume. Moduli related to strains that distort the registry of the (111) planes were observed to increase with increasing registry or coherency. The largest increase in moduli observed was a 21% increase in the modulus C_{yxyx} for the coherent multilayer relative to pure Pd. The maximum increase due to coherency was the 13% increase in bulk modulus calculated for the coherent multilayer relative to the incoherent multilayer.

(3) The results of this study were related to the coherency and interface stress models for the supermodulus effect. Two differences with the coherency model were observed. First, compressive strains in the coherent lattice (-1.5%) were much less than tensile strains (5.5%), and the coherency model assumes approximately equal strains. Secondly, the biaxial modulus was a minimum for the coherent lattice rather than a maximum, although other moduli were maximized. The interface strain models predict, in agreement with this study, that the biaxial modulus increases when the interface becomes incoherent, but the effect was very small in this system (7% increase). The interface strain models assume that elastic moduli of multilayers increase as the spacing between planes normal to the layer decrease. A large decrease in interplanar spacing normal to the (111) layers was observed for the coherent lattice, but the biaxial modulus for this multilayer was observed to decrease.

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