

## Application of the embedded-atom method to liquid transition metals

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The recently developed embedded-atom method (EAM) of Daw and Baskes [Phys. Rev. B **29**, 6443 (1984); Phys. Rev. Lett. **50**, 1285 (1983)] is applied to the description of liquid transition metals. A particular set of EAM functions fitted to bulk *solid* properties is then used to compute the static structure factor and theoretical pressure at the experimental zero-pressure density of various liquid transition metals. The results are in good agreement with experimental data, thus supporting the overall validity of the approach. Further, a systematic prescription for the determination of approximate pair potentials, as well as three- or more-body interactions, from the EAM formalism is presented and shown to give results for the pair correlations in good agreement with the full theory. Finally, the numerical values of the EAM functions used in the calculations for Ni, Pd, Pt, Cu, Ag, and Au are given.

### I. INTRODUCTION

There is a great deal of interest in modeling the energetics of transition metals. For ideal crystalline solids, various band-structure techniques are available. Unfortunately, the band-structure approach requires a periodic system, so it is not suitable for the study of complex defects or amorphous systems. As an alternative that can be used in these cases, pair-potential models have received a great deal of attention.<sup>1-5</sup> However, these approaches require large volume-dependent terms representing the energy of the electron gas and the structure-independent portion of the electron-ion interactions.<sup>6</sup> It is not clear how these contributions should be treated near extended defects and surfaces.

Recently, Daw and Baskes<sup>7,8</sup> have proposed a new framework for calculating the energetics of transition metals which they call the embedded-atom method (EAM). In this approach the dominant energy of the metal is viewed as the energy to embed an atom into the local electron density due to the remaining atoms of the system. This is supplemented by a short-range core-core repulsion. The resulting approach combines the computational simplicity needed for defects and amorphous systems with a physical picture which includes many-body effects and avoids the ambiguities of the pair-potential schemes. This method has been applied in the solid phase to such problems as defects, surfaces, alloys, impurities, and fracture.<sup>7-9</sup> It has also been used to study the high-coverage behavior of hydrogen on transition-metal surfaces.<sup>10</sup>

In this paper the EAM will be used to study the structure and energetics of the liquid state of some pure-transition metals. There are two motivations for this work. First, the liquid state is qualitatively different from the other applications of the method to date and so will provide a critical test of the range of applicability of the method as well as the empirical procedures used to determine the EAM functions. Second, the structural properties of the liquid metals are of inherent interest. In particular, the theory of the liquid state has developed to the

point that the pair structure can be easily calculated given a pair-interaction description of the energetics.<sup>11-13</sup> Therefore, even for systems in which many-body interactions may be important, such as the transition metals, it is still useful to find effective pair interactions. Note that these interactions are generally density dependent<sup>14</sup> because of the changes in the electronic structure with density and because of the average effects of any three- or more-body interactions. In this paper, we will show how an effective pair interaction for the liquid state can be derived from the EAM. These effective interactions depend on the overall density. Thus this approach provides a simple way to determine the density dependence of the optimum effective interactions.

### II. THEORY

Within density-functional theory the energy of a system of atoms for a given arrangement of the atomic nuclei can be written as a unique functional of the total electron density. If one assumes that this functional is semilocal in nature, i.e., depends only on the local electron density and its derivatives, and that the contribution to the electron density at an atom due to the remaining atoms of the system is slowly varying, one can argue that the major contribution to the energetics is the energy to embed the atom into the electron density of the neighboring atoms.<sup>15</sup> This energy is supplemented by a short-range doubly screened pair interaction that accounts for the core-core repulsions. These ideas have been developed in detail by Daw and Baskes,<sup>7,8</sup> who argue that the total energy of the system can be written as

$$E_{\text{tot}} = \sum_i F_i(\rho_{h,i}) + \frac{1}{2} \sum_{i,j} \phi_{ij}(R_{ij}). \quad (1)$$

In this expression,  $\rho_{h,i}$  is the total electron density at atom  $i$  due to the host, i.e., the rest of the atoms in the system, and  $F_i$  is the embedding energy for placing an atom into that electron density. Finally,  $\phi_{ij}$  is a short-range pair interaction representing the core-core repulsion, and  $R_{ij}$  is

the separation of atoms  $i$  and  $j$ .

In order to apply this formalism, a model is needed for the host electron density. A simple, yet reasonably accurate approximation is the superposition of atomic densities:

$$\rho_{h,i} = \sum_{j (\neq i)} \rho_j^a(R_{ij}). \quad (2)$$

In this expression,  $\rho_j^a(R)$  is the atomic electron density of atom  $j$  at the distance  $R_{ij}$  from the nucleus. This choice for the electron density makes the actual calculations with this method not significantly more computer intensive than the use of pair-potential models.

The other ingredient needed by the theory are the embedding functions and pair interactions. The embedding function can be obtained for low- $Z$  atoms from local-density calculations of the energy of an atom placed in jellium. However for higher  $Z$  such calculations are not feasible though the qualitative form of  $F$  should be the same as for the small- $Z$  elements. The embedding energy  $F(\rho)$  should start at zero for zero density, decrease to a simple minimum, and then increase for larger electron density. The minimum of  $F(\rho)$  should occur for  $\rho$  slightly greater than the average electron density seen in the equilibrium solid with the depth of the minimum somewhat greater than the bulk sublimation energy. The pair-potential term in this model should be short-range and purely repulsive. (The binding in this picture comes from the embedding energy.)

The embedding functions are determined by choosing functional forms meeting these general requirements and by adjusting them to describe the bulk equilibrium solid. In particular, they are fitted to the equilibrium lattice constant, heat of sublimation, elastic constants, vacancy-formation energy, and bcc-fcc energy difference. The details of the fitting procedure are described by Daw and Baskes<sup>8</sup> and the parameterizations of the particular functions used in these calculations<sup>16</sup> are presented in the Appendix.

Note that in the determination of the embedding function and the pair potential, only information about small deviations from the equilibrium *solid* are used. Therefore it is not clear that these functions will reasonably describe a system, like the liquid, that is qualitatively different from the solid. In particular, the average electron density seen by each atom in the liquid is less than in the solid because of the lower overall atomic density. Thus the liquid-state calculations provide a test of the form of the embedding function at lower than usual electron densities. Also, the motion of the atoms in the liquid brings them much closer together at times than is found in the equilibrium solid. Thus the pair-correlation function of the liquid provides a sensitive test of whether the functional form used for  $\phi$  is accurate for distances less than the nearest-neighbor distance in the solid. Thus the liquid-state calculations provide a test of the functional form. (The forms used here are described in the Appendix.) Conversely, the liquid data can be used to improve the choice of the functional forms.

It should also be noted that this formalism does not incorporate the thermal excitation of the electronic degrees

of freedom. The total-energy expression in Eq. (1) gives the electronic ground-state energy for the given ionic arrangement. [There is an adiabatic approximation implicit in the derivation of Eq. (1), as is usual for the calculation of the energetics of metallic systems.] Since this method gives no information about the electronic density of states of the metal, it cannot predict the energy of the thermal electronic excitations. Thus this method by itself cannot be used to compute the internal energy of the liquid metal. However, since the variation of the electronic energy with atomic position should be only weakly dependent on the temperature for temperatures well below the Fermi energy, the ionic motion and energies should be well represented by this approach. Further, simple estimates based on the free-electron model for the contribution of the electronic excitations to the pressure show that it should be only a few kbar. Thus this contribution to the pressure will be ignored in the calculations below.

### III. COMPUTER SIMULATIONS

Since the EAM energy implicitly includes many-body terms, the well-developed theory of liquids interacting with pair potentials cannot be used. Thus molecular-dynamics computer simulations have been performed to determine the predictions of the EAM for the liquid structure and pressures. The simulations consider a cubic cell of 500 atoms with periodic boundary conditions. After an equilibration period, a histogram of atomic separations is produced in order to compute the pair-correlation function<sup>12</sup>  $g(r)$ . The experimentally measurable structural information is the static structure factor. This is related to  $g(r)$  by

$$S(k) = 1 + n \int [g(r) - 1] e^{ik \cdot r} d^3r. \quad (3)$$

Here  $n$  is the atomic number density and the integration is over all space. In order for the Fourier transform to be evaluated accurately,  $g(r)$  is needed at distances larger than can be measured in the simulation because of the finite size of the simulation cell. The required extension has been obtained by a variation of a method due to Verlet<sup>17</sup> based on the direct correlation function. The direct correlation function  $c(r)$  is defined by the relation

$$h(r) = c(r) + n \int c(r') h(\mathbf{r} - \mathbf{r}') d^3r', \quad (4)$$

where  $h(r) = g(r) - 1$ . The direct correlation function is known to be very small for distances greater than the range of the interparticle interactions.<sup>18</sup> For the parameterization used here, the atomic densities and pair repulsions are negligible by 6 Å and so we assume that  $c(r) = 0$  for  $r > 6.5$  Å. For  $r < 6.5$  Å, the value of  $h(r)$  is known from the simulation. These constraints along with Eq. (4) determine  $g(r)$  for all  $r$  and allow the reliable determination of the structure factor.

The pressure of the system can be obtained from the general expression<sup>12</sup>

$$P = nk_B T - \left\langle \frac{\partial E}{\partial V} \right\rangle. \quad (5)$$

In this expression,  $E$  is the internal energy of the system,  $V$  is the volume, and the derivative refers to the change in

energy due to a uniform expansion of the system. The angular brackets refer to an average computed at constant number of particles and temperature. For the EAM this expression yields the following result for the pressure:

$$P = nk_B T - (n/3N) \left\langle \sum_{\substack{i,j \\ i \neq j}} [F'_i(\rho_{h,i}) \rho_j^{a_i}(R_{ij}) + \frac{1}{2} \phi'(R_{ij})] R_{ij} \right\rangle, \quad (6)$$

where  $N$  is the total number of particles,  $R_{ij}$  is the separation of atoms  $i$  and  $j$ , and the primes denote differentiation with respect to the argument.

Simulations have been performed for the following metals: Cu, Ag, Au, Ni, Pd, and Pt. In all cases the density and temperatures were chosen to be close to the melting points of the metals. (For the cases where experimental structure data are available, the conditions were chosen to correspond to the experimental conditions.) Table I lists the temperatures and densities used in the calculations along with the resulting pressures and internal energies relative to the atomic state. Figures 1–4 present the static structure factors computed for Cu, Ag, Au, and Ni along with the experimental x-ray diffraction results of Waseda and Ohtani.<sup>19</sup> No experimental data for Pd and Pt could be found. The structure factors computed here for those metals are very similar to the other four.

The agreement between theory and experiment for the structure factor is quite good and is comparable to the agreement between different experimental determinations of the structure factor.<sup>20</sup> The pressures obtained are generally negative with a magnitude of about 10–20 kbar. However, that pressure is fairly small compared to the typical bulk moduli of 1 Mbar. The magnitude of the computed pressures indicate that the equilibrium zero-pressure densities will be within about 1% or 2% of the experimental values. Simulations performed for slightly different densities confirm this.

This level of agreement is quite encouraging considering that the input data to the model are from the solid state. The liquid samples a very different distribution of interparticle separations, especially at short distances. Thus a method fit only to solid data need not give reasonable results for the liquid state. In particular, while the pair-potential model of liquid Ni proposed by Baskes and Melius<sup>5</sup> gives a good description of the solid state, the

TABLE I. The pressure and internal energy per atom for the liquid metals as computed by the computer simulations using the EAM for the temperatures and atomic densities specified.

Element	$T$ (K)	$n$ ( $\text{\AA}^{-3}$ )	$P$ (kbar)	$E/N$ (eV)
Ni	1775	0.0792	-28.4	-3.72
Pd	1825	0.0595	-17.4	-3.18
Pt	2045	0.0584	-22.3	-4.95
Cu	1420	0.0755	-8.6	-2.99
Ag	1270	0.0517	-17.2	-2.33
Au	1420	0.0526	-3.3	-3.38

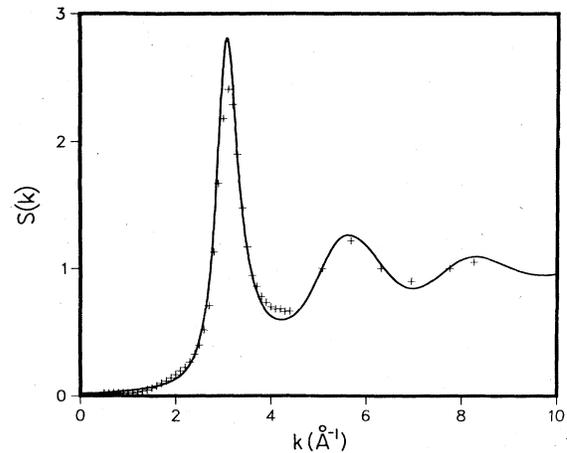


FIG. 1. Static structure factor  $S(k)$  for liquid Ni at  $T=1775$  K and  $n=0.0792 \text{ \AA}^{-3}$ . The solid line is the EAM result and the points are the experimental data (Ref. 19).

structure factor that we obtain for that pair potential is in very poor agreement with the experimental values. [The amplitude of the first maximum of  $S(k)$  exceeds 3.8 with the subsequent oscillations also much larger than experiment.] This problem is inherent in any parametrization that is based solely on solid data. Thus the calculation of liquid-state properties provides a crucial test of the applicability of both the basic model as well as the parametrization of the functions in the model.

#### IV. PAIR-POTENTIAL APPROXIMATION

While it is known that many-body interactions are not negligible in transition metals, the approximation of the energetics by pair potentials is frequently useful since the statistical mechanics of the pair-potential liquid are well understood. Therefore we have developed a systematic procedure for extracting effective pair and three- or more-body interactions from the EAM. A major advantage of this formulation is that the pair forces are automatically state dependent in that they depend on the

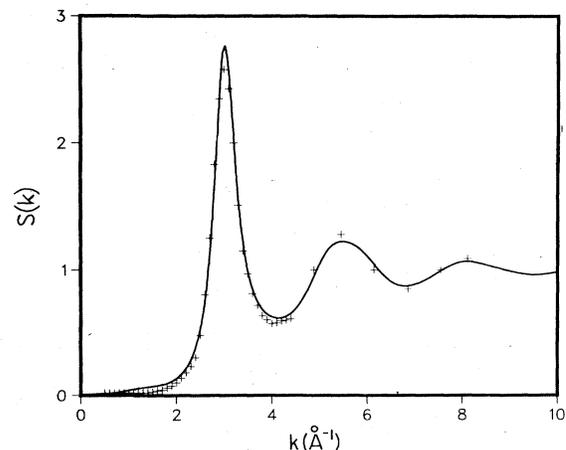


FIG. 2. Static structure factor  $S(k)$  for liquid Cu at  $T=1420$  K and  $n=0.0755 \text{ \AA}^{-3}$ . The solid line is the EAM result and the points are the experimental data (Ref. 19).

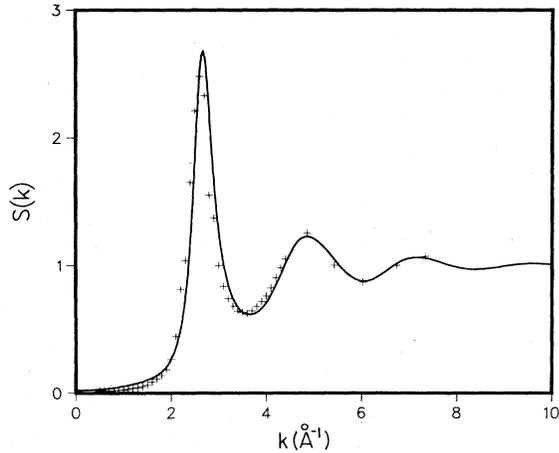


FIG. 3. Static structure factor  $S(k)$  for liquid Ag at  $T=1270$  K and  $n=0.0517 \text{ \AA}^{-3}$ . The solid line is the EAM result and the points are the experimental data (Ref. 19).

overall density of the system. In this way the average effects of the three- or more-body terms in a rigorous energy expansion are included in the effective-pair terms in a way that is appropriate for the density of the system in question. The formulation also permits the extraction of higher-order terms so one can check whether a pair approximation is reasonable.

To derive a pair and three- or more-body interaction expansion from the EAM energy, we need only look at the embedding energy since the core-core repulsion term is already in the desired form. The basic approach is to replace  $F(\rho)$  with a Taylor-series expansion about the average host electron density  $\bar{\rho}$ . To this end the electron density at site  $i$  will be written

$$\rho_{h,i} = \bar{\rho} + \sum_{j \neq i} [\rho_j^a(R_{ij}) - \delta], \quad (7)$$

where  $\delta = \bar{\rho}/(N-1)$ .  $N$  is the number of atoms in the

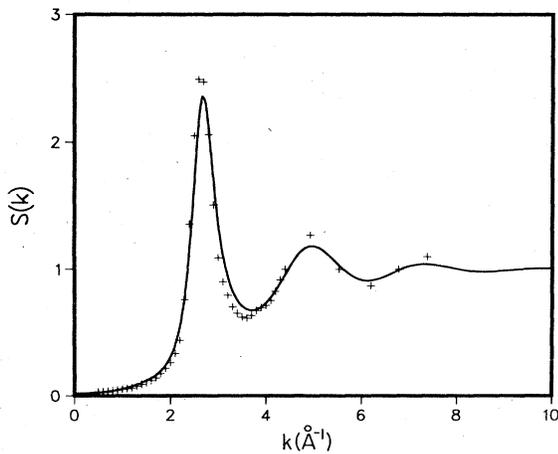


FIG. 4. Static structure factor  $S(k)$  for liquid Au at  $T=1420$  K and  $n=0.0526 \text{ \AA}^{-3}$ . The solid line is the EAM result and the points are the experimental data (Ref. 19).

system. If one now keeps terms in the Taylor expansion through second order, one can obtain the following expression for the embedding energy:

$$\begin{aligned} \sum_i F(\rho_{h,i}) = & NF(\bar{\rho}) + \sum_{\substack{i,j \\ j \neq i}} F'_i(\bar{\rho})[\rho_j^a(R_{ij}) - \delta] \\ & + \frac{1}{2} \sum_{\substack{i,j \\ j \neq i}} F''_i(\bar{\rho})[\rho_j^a(R_{ij}) - \delta]^2 \\ & + \frac{1}{2} \sum_{\substack{i,j,k \\ k \neq j \neq i \neq k}} F''_i(\bar{\rho})[\rho_k^a(R_{ik}) - \delta][\rho_j^a(R_{ij}) - \delta]. \end{aligned} \quad (8)$$

The summation in the last term avoids coincidence of any two of the summation indices. Also,  $F'$  and  $F''$  represent the first two derivatives of the embedding energy of atom  $i$  with respect to electron density evaluated at  $\bar{\rho}$ . The first term here represents the simplest approximation to the total embedding energy. The next two terms give pair-potential-like contributions to the embedding energy in that they involve a double sum over pairs of atoms. The final term represents the three-body contributions. The purpose of writing the change of density in the form of Eq. (7) is so that if the perturbation involved averages to zero over the entire system, then the three-body term vanishes. This leads to a sensible separation of the two- and three-body parts of the second-order term in the Taylor series.

The last step in the evaluation of the pair potential is the removal of the quantity  $\delta$  from the expression. Note that many of the terms involving  $\delta$  in Eq. (8) do not scale with  $N$ . These terms are negligible in the thermodynamic limit,  $N \rightarrow \infty$ , and so can be dropped. If we choose to ignore three-body interactions, the last term in Eq. (8) should also be dropped. The EAM energy can then be approximated by

$$E_{\text{tot}} \approx N[F(\bar{\rho}) - \bar{\rho}F'] + \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \psi(R_{ij}), \quad (9)$$

where the pair potential  $\psi$  is given by

$$\psi(R) = \phi(R) + 2F'(\bar{\rho})\rho^a(R) + F''(\bar{\rho})[\rho^a(R)]^2. \quad (10)$$

Note that the above expression is written for a single-component system. The generalization to a multicomponent system is straightforward provided one makes all expressions properly symmetrized with respect to the particle types.

The above general procedure can be extended to higher orders to define a hierarchy of  $n$ -body interactions. The lowest-order three-body term is the last term in Eq. (8). However, note that the inclusion of this three-body term will also modify the one- and two-body terms when the product is expanded. This results from the use of Eq. (7) to describe the electron-density variations. For the optimum effective pair interaction the higher-body terms that are discarded should be as small as possible. The above separation achieves this since the three-body term vanishes if  $\sum_j \rho_j^a = \bar{\rho}$ , which will be approximately correct for each atom. Thus the one- and two-body terms that re-

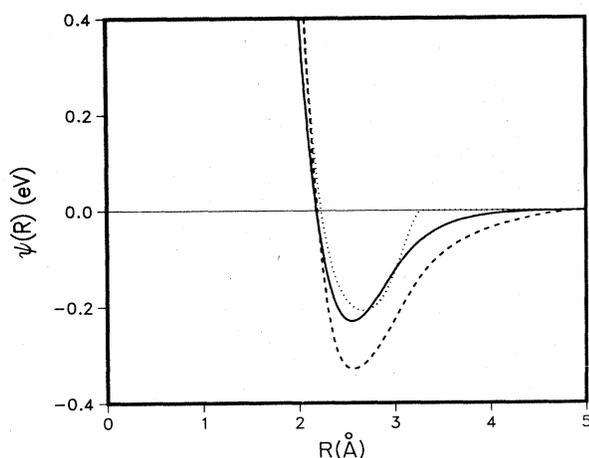


FIG. 5. Effective pair potential for liquid Cu computed from Eq. (10) (solid line) and the empirical pair potentials due to Baskes and Melius (Ref. 5) (dashed line) and to Johnson (Ref. 21) (dotted line).

sult from expanding the last term of (8) are only appropriate if the corresponding three-body interaction is included in the energy. Without that three-body interaction, those one- and two-body terms will lead to a less accurate description of the energy at the pair level.

The last quantity needed to apply this prescription for the pair potentials is the average host electron density for an atom in the liquid,  $\bar{\rho}$ . This can be computed from the atomic electron densities and the pair-correlation function of the liquid by the equation

$$\bar{\rho} = n \int \rho^a(r) g(r) d^3r. \quad (11)$$

However,  $g(r)$  is generally not available before one has computed the pair interactions. Fortunately, the pair interactions are not strongly dependent on the exact value of

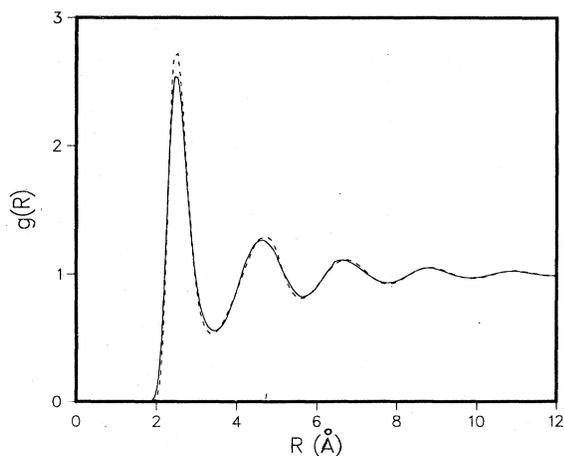


FIG. 6. Comparison of the pair-correlation function  $g(R)$  for liquid Cu as computed from the computer simulation using the full EAM (solid line) and from the effective pair potential (dashed line).

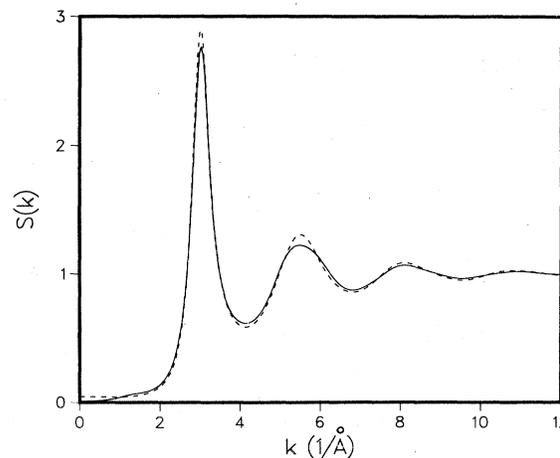


FIG. 7. Comparison of the static structure factor  $S(k)$  for liquid Cu as computed from the computer simulation using the full EAM (solid line) and from the effective pair potential (dashed line).

$\bar{\rho}$ . Therefore, we approximate  $\bar{\rho}$  by the average electron density for a fcc solid with a lattice constant such that the overall atomic density matches the liquid-state density. Since this determines the interatomic separations,  $\bar{\rho}$  can be readily computed from the superposition approximation.

The pair potential determined in this manner for liquid Cu at its melting point is shown in Fig. 5. Note that the potential has a simple shape with no long-range oscillations. For comparison the empirical pair potentials determined by Baskes and Melius<sup>5</sup> and by Johnson<sup>21</sup> are also included in Fig. 5. The pair-correlation function  $g(r)$  and the static structure factor  $S(k)$  have both been computed from the pair potential [Eq. (10)] in conjunction with the modified hypernetted-chain equation as described by Lado *et al.*<sup>11</sup> The results are compared with the full simulation in Figs. 6 and 7. The comparisons for the other elements considered here are very similar. In all cases the pair approximation predicts a slightly larger exclusion region at small separations than the full EAM, but overall the agreement is quite encouraging. Note that the disagreement between the pair and simulation results is larger than the typical errors arising from the use of the modified hypernetted-chain equation to calculate the liquid structure.<sup>11,18</sup> Therefore the differences do reflect

TABLE II. Parameters used to define the atomic electron densities and pair potentials used in these calculations. See Appendix for definitions.

Element	$N_s$	$a_1$	$a_2$	$R_c$
Ni	0.86	0.070 937	0.146 031	3.0045
Pd	0.67	0.124 715	0.041 904	3.3203
Pt	0.96	0.065 699	0.110 951	3.3459
Cu	1.05	0.140 974	0.017 517	3.0899
Ag	1.3359	0.132 594	0.000 000	3.4825
Au	0.8454	0.105 499	0.007 250	3.4739

TABLE III. Values of the embedding function  $F(\rho)$  and corresponding spline knots used in these calculations. The energies are in eV and the electron densities are in  $\text{\AA}^{-3}$ .

$\rho$	$F(\rho)$	$\rho$	$F(\rho)$	$\rho$	$F(\rho)$
Ni		Pd		Pt	
0.0	0.0	0.0	0.0	0.0	0.0
0.014 46	-3.5847	0.007 83	-3.1560	0.011 40	-4.5793
0.028 91	-5.1449	0.015 67	-4.7725	0.022 80	-6.5328
0.057 83	-3.4041	0.031 33	-3.0832	0.045 60	-3.8272
0.066 50	0.0	0.036 03	0.0	0.524 45	0.0
Cu		Ag		Au	
0.0	0.0	0.0	0.0	0.0	0.0
0.013 70	-2.9239	0.010 48	-2.4085	0.007 28	-3.2170
0.027 40	-4.2953	0.020 96	-3.6969	0.014 55	-4.6278
0.054 81	-2.8523	0.041 92	-2.5425	0.029 10	-2.7699
0.063 03	0.0	0.048 21	0.0	0.033 47	0.0

shortcomings of the pair-potential model. However, these results show that pair potentials deduced from Eq. (10) provide a realistic description of the pair correlations in the liquid state.

### V. CONCLUSION

These calculations have shown two points. First, the embedded-atom method provides a realistic description of the pair correlations as well as the pressure of liquid metals. These calculations were performed for functions fit only to solid data. Since the liquid state samples  $F(\rho)$  and  $\phi(R)$  in different regimes than the solid, it should be possible to improve the functional forms to obtain a better description of the liquid and still describe the solid accurately. This work is in progress. These results do show that the EAM formalism is capable of providing a good description of the liquid state. The second major result is a simple prescription for determining an effective pair-potential approximation to the full EAM energy. This simplification has been shown to work well for predicting the static structure factor of the liquid and so may be of use in other situations which are dominated by the pair forces.

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### APPENDIX

This appendix describes the parametrization of the particular functions used in these calculations.<sup>16</sup> The three

quantities needed for the numerical implementation of the EAM are the atomic electron densities, pair potentials, and embedding functions. The atomic electron densities are obtained from the Hartree-Fock calculations of Clementi and Roetti<sup>22</sup> and of McLean and McLean.<sup>23</sup> As discussed in Ref. 8, the appropriate atomic configuration for the condensed state is not known. Here the occupancy of the outer  $s$  orbital is fitted to the hydrogen heat of solution in the various materials. The atomic density is then written in the form

$$\rho^a(R) = (N - N_s)\rho_d^a(R) + N_s\rho_s^a(R),$$

where  $N$  is the total number of outer electrons,  $N_s$  is a measure of the  $s$  electron content of the atomic density,  $\rho_s^a$  is the density of the outer  $s$  orbitals, and  $\rho_d^a$  is the density of the outer  $d$  orbitals. The wave functions used to calculate these densities are for the atomic configuration with a filled outer  $s$  shell. The  $N_s$  values for the various elements are listed in Table II.

The pair potential is expressed in terms of an effective charge  $Z(R)$  such that  $\phi(R) = Z^2(R)/R$ . The effective charge is parametrized by the simple polynomial form

$$Z^2(R) = a_1(R_c - R)^3 + a_2(R_c - R)^4$$

for  $R < R_c$  and is zero otherwise. The values of  $a_1$ ,  $a_2$ , and  $R_c$  are listed in Table II. Distances are expressed in angstroms and  $Z(R)$  is expressed in units of electron charge.

The embedding energies are described by natural splines. The knots used for the spline and the corresponding values of  $F(\rho)$  are given in Table III. Note that we use the usual convention for spline interpolation of setting the curvature of the spline fit to zero at the endpoints. The electron densities are in units of inverse  $\text{\AA}^3$  and the energies are in electron volts (eV).

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