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LETTERS TO THE EDITOR

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NOTES

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In recent papers,[1,2] we used the Voter and Chen (VC) version of the embedded atom model (EAM) (Ref. 3) in conjunction with molecular dynamics (MD) to compute the diffusion constants D and shear viscosities η of the face-centered-cubic (fcc) transition metals Ni, Pd, Pt, Cu, Ag, and Au in the liquid phase. The VC EAM differs from other EAM approaches (in particular, from that of Foiles, Baskes, and Daw[4]) in two main ways: (a) The core–core pair interaction has a medium-range attractive contribution, rather than being entirely repulsive; and (b) properties of the diatomic molecule as well as bulk solid-state properties were used in fitting the embedding function and pair interaction. The good general agreement between the VC EAM predictions of Refs. 1 and 2 and available experimental data[5] is quite encouraging taking into account that liquid-state properties were not used in fitting the EAM functions, and suggests that this model (and probably other EAM approaches) may also be capable of describing reasonably well the transport coefficients of binary liquid alloys including at least one transition metal. Extensive comparison between simulated and experimental data for the transport coefficients of this kind of system is not possible at present, but such comparisons can be made in the case of liquid Ni–Al, for which there is both an appropriate EAM potential[3] and enough experimental data[6] for comparison with theoretical predictions.

This paper describes an EAM MD study of the diffusion coefficient D_{Ni} of Ni impurity in liquid Al. Experimental values of this property have been reported by Ejima *et al.*[6] for several temperatures. The EAM model used in our calculations was that proposed by Voter and Chen,[3] which was optimized by its authors for prediction of the elastic constants and vacancy formation energies of pure Ni (fcc) and pure Al (fcc), the bond lengths and bond energies of the diatomic molecules Ni_2 and Al_2, the lattice constant, cohesive energy, elastic constants, vacancy formation energy, antiphase boundary energies, and superlattice intrinsic stacking fault energy of Ni_3Al ($L1_2$), and the lattice constant and cohesive energy of the $B2$ phase NiAl. The use of the properties of the diatomic molecules among the data to which the EAM is fitted makes the VC Ni–Al potential particularly appropriate for describing the properties of Ni–Al clusters, as was shown in Ref. 7. Below we sketch the computational procedure used in this work to compute the diffusion coefficient D_{Ni} in liquid Ni–Al alloys, and we then present our results.

Using the VC EAM Ni–Al potential, we performed MD simulations of a system comprising 3 Ni atoms and 497 Al atoms at the temperatures listed in Table I (densities were considered to be those reported by Waseda[8] for pure liquid Al at the temperatures specified). The relative proportions of Ni and Al atoms were taken so as to allow comparison with the experimental D_{Ni} data reported by Ejima *et al.*[6] The computational procedure was as follows. First, at the chosen temperature and density, we performed a canonical MD simulation using the Nosé constant temperature technique,[9] the equations of motion being solved using a fourth-order Gear predictor-corrector algorithm[10] with a time step of 10^{-4} ps. The initial configuration was obtained by melting an fcc structure. The energy of the system was calculated over 10^4 time steps after an appropriate initial equilibration period. Then, starting from a configuration with an energy very close to the average value obtained previously, microcanonical MD simulations were performed using the velocity Verlet algorithm[10] with a time step of 2×10^{-3} ps. After an appropriate equilibration period, a configuration was recorded every 0.01 ps. In order to be able to estimate the statistical uncertainty of the results of these microcanonical simulations, the properties of interest were averaged over six successive runs of 25×10^3 time steps. The diffusion constant D_{Ni} was calculated from the mean square displacement using

TABLE I. Values of the diffusion coefficient D_{Ni} of Ni impurity in liquid Al at the temperatures specified, as computed using the Einstein (E) and Green–Kubo (GK) relations and as obtained experimentally (Ref. 6). All values in $\mathrm{Å}^2\ \mathrm{ps}^{-1}$.

	E	GK	Expt.
$T=1091$ K	0.55 ± 0.05	0.55 ± 0.05	0.567 ± 0.076
$T=1250$ K	0.76 ± 0.04	0.76 ± 0.03	0.769 ± 0.081

the Einstein formula and from the velocity autocorrelation function using the Green–Kubo relation.[10,11]

In Table I we compare the results of our calculations with the experimental data reported in Ref. 6. For both the temperatures considered, the agreement between the simulated and experimental values of D_{Ni} is excellent. This may be considered as a test of the description of transport properties of liquid binary alloys by EAM potentials parametrized without reference to liquid-state properties.

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