Improved numerical results for the three-dimensional alloy with site diagonal disorder*

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Densities of states are obtained for ~ 10000-atom three-dimensional alloy models with site-diagonal disorder, and the results are compared with the single-site coherent-potential approximation. The numerical approach contains several improvements over our previous calculations.

Recently, we presented some exact numerical results for finite model alloy systems with site-diagonal disorder.[1] These results were used to verify the accuracy of single-site coherent-potential approximation (CPA) calculations for corresponding infinite alloy lattices. Since these calculations were presented, several improvements have been made in the numerical method which we used.[2] First, we have found that by averaging over models of different sizes, certain spurious structure due to finite size effects is considerably reduced. Second, in using the equation-of-motion method, we have found that it is better to use a Gaussian broadening function rather than the Lorentzian used in our previous work. Taken together, these advances give a significant improvement in the quality of the finite model results.

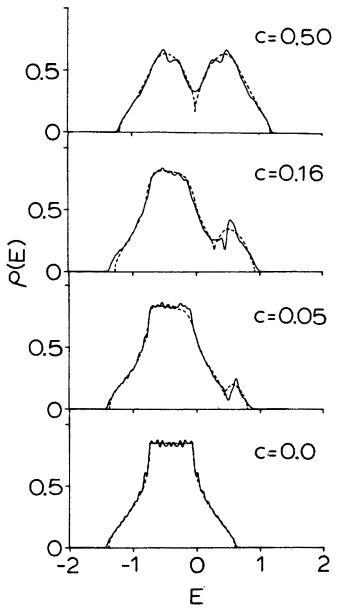

FIG. 1. Density of states for four concentrations c of type-A atoms for $\delta = 0.8$. Solid curves give the numerical results for averages of eight finite models. Broken curves are CPA results.

In Fig. 1, we give an improved version of the results of Fig. 1 of Ref. 1 for the disorder parameter $\delta = 0.8$. This corresponds to site energies of $+0.4$ for the A atoms and -0.4 for the B atoms. The concentration of A atoms is denoted by c. The hopping integral is taken as $\frac{1}{6}$ so that the unperturbed bandwidth is 2 units for this simple cubic structure. (See Ref. 1 for further details of the model system.) Each of the solid curves represents an average over eight different random alloy models, four of dimensions $16 \times 20 \times 24$, and four of dimensions $18 \times 22 \times 26$. The resolution width is 0.04 units. We estimate that these finite model results are within 3% of those for the corresponding infinite alloys for regions where $\rho(E) \gtrsim 0.5$. The fractional error due to statistical effects varies approximately as $[\rho(E)]^{-1/2}$. The broken curves are CPA results.

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