Ching Replies: The preceding Comment by Muir[1] on our recent Letter[2] raised the question of accuracy in the calculation of thermopower S for the a-$Mn_{75}Zn_{25}$ metallic glass. He pointed out that the experimental value of S for this glass should be $-0.2\ \mu V/K$ instead of $-0.8\ \mu V/K$ cited in our Letter. Muir is correct in pointing out that in a free-electron-like glass, the disorder scattering completely dominates and the effect of electron-phonon scattering is negligible; and as such, we should expect a better agreement for a-$Mg_{75}Zn_{25}$ than other strong scattering glasses. However, from the standpoint of a theoretical calculation, the evaluation of S for a-$Mn_{75}Zn_{25}$ is the most difficult. S is calculated according to the following expression:

$$S(T)=\frac{1}{\sigma(T)}\frac{k}{e}\int_{-\infty}^{\infty}\langle\sigma_E\rangle\frac{E-E_F}{kT}\left[\frac{\partial f(E)}{\partial E}\right]dE\,,$$

where σ_E is the conductivity function. It is apparent that S is very sensitive to the shape and the curvature of σ_E near the Fermi level E_F. The small S value for a-$Mn_{75}Zn_{25}$ is reflected in the rather flat σ_E near E_F [see Fig. 3(b) of Ref. 2]. To a large extent, the accuracy of σ_E is determined by the statistics of the calculation, i.e., the number of states in the vicinity of E_F that were included in the calculation. The density of states (DOS) at E_F for a-$Mg_{75}Zn_{25}$ is very low as illustrated in the figure,[3] typical of a free-electron-like glass. For strong scattering systems involving d electrons, the DOS at E_F is usually much higher and σ_E can be evaluated more accurately because of the improved statistics. To improve the statistics for a-$Mg_{75}Zn_{25}$ to the same level as a-Ni, calculations with models containing 500–1000 atoms may be needed.

Our Letter[2] advocates for a first-principles real-space approach for the theory of metallic glasses. It is demonstrated that such an approach can be applied to different types of metallic glasses with good results in electronic and transport properties. I certainly feel very gratified that even for the computationally most difficult system

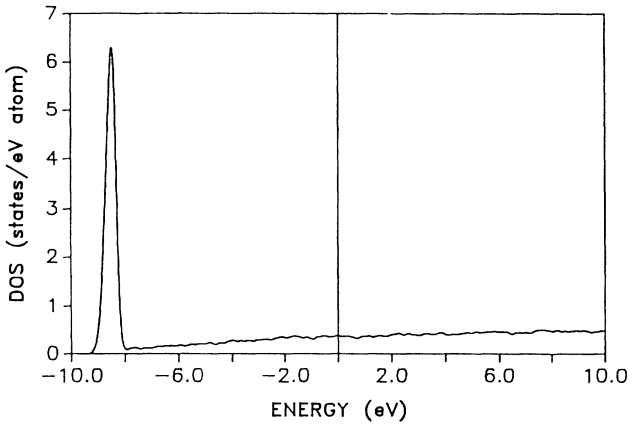

FIG. 1. Density of states of a-$Mg_{75}Zn_{25}$. The sharp peak at -8.6 eV corresponds to the corelike Zn $3d$ states.

a-$Mg_{75}Zn_{25}$, we had obtained a thermopower value with the correct sign and the order of magnitude, and this value can be further improved by larger-scale computations. This is far more significant than some other approaches which claim "exact" agreement, albeit with arbitrarily chosen parameters.

W. Y. Ching
Department of Physics
University of Missouri-Kansas City
Kansas City, Missouri 64110

Received 26 June 1989
PACS numbers: 71.25.Mg, 72.15.Cz

[1]W. B. Muir, preceding Comment, Phys. Rev. Lett. **64**, 1180 (1990).

[2]Guang-Lin Zhao and W. Y. Ching, Phys. Rev. Lett. **62**, 2511 (1989).

[3]Guang-Lin Zhao, Yi He, and W. Y. Ching (to be published).