Comment on "Microscopic Real-Space Approach to the Theory of Metallic Glasses"

In a recent Letter Zhao and Ching[1] used a real-space approach to calculate the properties of metallic glasses. In particular, they calculate the electrical resistivity ρ and the thermopower S of $Cu_{60}Zr_{40}$, $Mg_{75}Zn_{25}$, and amorphous Ni. The calculation ignores the effects due to phonons which may be significant for resistivity where very accurate measurements are possible but which should be insignificant in the thermopower. This can easily be seen using the Nordhiem-Gorter relation for the thermopower due to different scattering mechanisms. In this case

$$S=\frac{\rho_p}{\rho_p+\rho_d}S_p+\frac{\rho_d}{\rho_p+\rho_d}S_d\,,$$

where the subscripts p and d refer to phonon and disorder scattering, respectively. In metallic glasses ρ_p is at most a few percent of ρ_d and hence S will be dominated by the disorder scattering. The experimental data used by Zhao and Ching appear to show good agreement between the calculated and measured thermopowers especially in the case of $Mg_{74}Zn_{25}$. Unfortunately the authors have chosen an incorrect value of -0.8 μV/K for the measured thermopower of this alloy.[2] The correct value is -0.2 μV/K at 160 K (Refs. 2 and 3) which makes the agreement between the measured and calculated thermopowers for $Mg_{75}Zn_{25}$ very poor. In many respects Mg-Zn alloys are among the simplest metallic glasses and the lack of agreement between the calculated and measured thermopower is most discouraging especially since the neglect of phonons in the calculation should be of little importance.

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Received 12 June 1989
PACS numbers: 71.25.Mg, 72.15.Cz

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