Shore and Rose Reply: We agree, in substantial part, with Soler's Comment [1] on the theory of ideal metals [2], our generalization of the electron gas. The uniform state of the ideal metal is, as noted by Soler and ourselves [3], metastable. Soler further considers dividing the background of the ideal metal into infinitesimally small pieces, and then compressing the system uniformly. He finds that although the first derivative of the energy is zero, the second derivative of the energy becomes negative for $r_s < 2.2$, and, consequently, that the system is unstable for smaller r_s's. This raises the question: Why were simple calculations based on the theory of ideal metals [2,3] so successful for the bonding energetics of metals? The division of the ideal metal into infinitesimal parts is a substantial idealization. It has the effect of making the Coulomb energy that would arise due to the overlap of the background charge zero. The Coulomb energy adds a finite positive contribution to the second derivative of the energy and tends to significantly stabilize the system if the background is divided into pieces on the size of an atom (or larger). For example, the second derivative of the energy with respect to an infinitesimal planar separation of the ideal metal into two half spaces remains positive for all $r_s > 1.20$.

The bulk moduli of the simple metals have also been calculated. In particular, we imagined dividing an infinite space of the equilibrium ideal metal (of the appropriate density) into atomic-size polyhedra on a bcc lattice; the background is kept rigid and uniform in each polyhedra. Upon compression the background densities of the polyhedra overlap. Our inputs were the r_s of the metal and the bonding valence [3]. The energy was calculated in second-order perturbation theory using the local-density approximation to density-functional theory. The lattice was uniformly compressed by a small amount, and the quadratic term in the energy change was evaluated. The resulting estimates for the bulk moduli are compared with the experiment in Fig. 1 and found to be in surprisingly close agreement. We note that Be, Al, and Zn have $r_s < 2.2$, the value at which Soler's instability sets in.

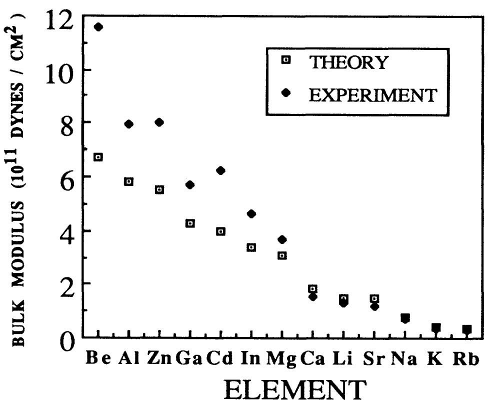

FIG. 1. Comparison of the bulk moduli calculated from the theory of ideal metals with experiment.

The calculations based on the ideal metal give accurate trends for the cohesive energies, the work functions, and the chemical potentials of the transition metals [3], but fail qualitatively for the surface energy and the bulk moduli of the transition metals. We attribute these failures to the instability noted by Soler. As Soler mentions, the stabilized jellium model of Perdew, Tran, and Smith [4] has a positive bulk modulus for all r_s's. We wish to comment on the differences between these very similar models. In Ref. [4], a compression of the metal is accomplished by changing the positive background density uniformly, with a consequent change in the Madelung energy. In our approach all departures from the equilibrium bulk metal, e.g., a uniform compression or other strain, a vacancy, a surface, etc., are generated in the same consistent manner: by displacing rigid ionic polyhedra. An attractive feature of our approach is that the theory provides a full model Hamiltonian for the valence electrons and is not tied to a density functional for the electron-electron interactions. The ideal metal is a substantially better starting point than jellium for a wide variety of first-principles many-body calculations as noted in Refs. [2,3]. These many-body calculations would appear to be much more difficult for a theory based on a density functional for the energy.

In short, the instability noted by Soler is inconsequential for the properties of the simple metals. However, it apparently leads to the failure to accurately predict the trends in the bulk moduli and possibly the surface energies of the transition metals.

Herbert B. Shore
Department of Physics
San Diego State University
San Diego, California 92182

James H. Rose
Ames Laboratory, U.S. Department of Energy
Iowa State University
Ames, Iowa 50011

Received 25 July 1991
PACS numbers: 71.10.+x, 71.45.Nt

[1] J. M. Soler, preceding Comment, Phys. Rev. Lett. **67**, 3044 (1991).

[2] Herbert B. Shore and James H. Rose, Phys. Rev. Lett. **66**, 2519 (1991).

[3] James H. Rose and Herbert B. Shore, Phys. Rev. B **43**, 11 605 (1991).

[4] J. P. Perdew, H. Q. Tran, and E. D. Smith, Phys. Rev. B **42**, 11 627 (1990).