

...nearly equal to the anisotropy of their short-range derivatives; (2) the bulk modulus is in all cases too large in relation to the shear constants; (3) the strain derivative of the bulk modulus is also too large compared to the derivatives of the shear constants; (4) these conditions appear more aggravated as one proceeds down the series from copper to silver to gold. These failures are present regardless of the specific form taken for the repulsive potential, as long as the potential is short-range in nature so that  $|r^3 W''''| > |r^2 W''''|$ . Effects (2), (3), and (4) lead one to suspect that the failure of conventional theory lies in the breakdown of the assumption that  $W$  depends on  $|r|$  only. This is, noncentral interactions could give a contribution to the shear constants, but would not of course contribute to  $\Omega B_{sr}$  and  $\Omega dB_{sr}/d \ln r$  because the latter are associated with volume strain alone in which no relative angular displacements occur.

TABLE VII. The elastic constants,  $\Omega C$ , and their hydrostatic strain derivatives,  $\Omega dC/d \ln r$ . The experimental values, the long-range contributions to each, and the difference between the experimental value and the long-range contribution to each, representing the short-range contribution is shown. The units are  $10^{12}$  erg atom $^{-1}$ .

Con- stant	Elastic constant			Hydrostatic strain derivative		
	Experiment	Long range	Short range	Experiment	Long range	Short range
B	16.8	4.5	12.3	-264	-32	-232
C	9.66	3.02	6.63	-111	-12	-99
C'	3.03	0.34	2.69	-27.4	-1.4	-26.0
B	18.3	3.5	14.8	-321	-24	-296
C	8.52	2.68	5.85	-120	-11	-109
C'	2.84	0.30	2.54	-33.2	-1.2	-32.0
B	29.3	3.5	25.7	-543	-25	-518
C	7.72	2.68	5.04	-151	-11	-140
C'	2.72	0.30	2.42	-37.0	-1.2	-35.8

\*The elastic constants used here are the values at 0°K. The copper values are taken from Overton and Gaffney (reference 23) and the gold values from Goens (reference 18). No low-temperature measurements have been made on silver, so the Bacon and Smith values (reference 17) were corrected to 0°K using the same fractional change which applied for the copper and gold results. These corrections were:  $C(0)/C(300)=1.084$ ,  $C'(0)/C'(300)=1.091$ ,  $B(0)/B(300)=1.036$ .

The last point suggests the procedure which has been adopted in order to carry the analysis further. We assume that the radial dependence of the short-range interaction is given by the two-parameter exponential potential  $W=A \exp(-pr/r_0)$ . The first row of Eqs. (14) then becomes

$$\Omega B_{sr} = \frac{2}{3} p^2 W, \quad \Omega dB_{sr}/d \ln r = -\frac{2}{3} (p+3) p^2 W. \quad (15)$$

These equations for the bulk modulus and its strain derivative serve to determine the parameters  $p$  and  $W$  for each of the metals when the appropriate values from Table VII are used. Numerical values for these parameters, describing the radial dependence of the short-range interaction, are entered in Table VIII. The values of the exponential parameter  $p$  for the three metals are found to be remarkably similar which suggests that the commonly used exponential form is quite a good one

TABLE VIII. Values of parameters describing the short-range interactions.  $W$  is the energy per bond of the radial interaction  $W=A \exp(-pr/r_0)$ . Closure failures, indicated by  $\Delta$ , are the amounts which must be added to conventional theory for the shear constants and their hydrostatic strain derivatives in order to obtain agreement with experiment. Units of all but  $p$  are  $10^{-12}$  erg atom $^{-1}$ .

	Cu	Ag	Au
$p$	16.0	17.1	17.1
$6W$	0.43	0.46	0.79
$\Delta(\Omega C)$	-0.81	-3.28	-10.9
$\Delta(\Omega dC/d \ln r)$	26.	53.	145.
$\Delta(\Omega C')$	0.11	-0.72	-3.29
$\Delta(\Omega dC'/d \ln r)$	16.	25.	64.

over a relatively wide range of ion-core overlap. We may take as a qualitative measure of the overlap the ratio of the ionic crystal radius to the metallic atomic radius, and these are 0.75, 0.87, and 0.95 for copper, silver, and gold, respectively. The numerical values of  $W$  are also reasonable,  $6W$  being about 10% of the latent heat of sublimation in each case.

The values of the exponential parameters  $p$  and  $W$  which have been obtained from the bulk modulus and its strain derivative may now be used to compute that portion of the shear stiffnesses, and of their hydrostatic strain derivatives, which arises in the radial dependence of the short-range interaction. Since we know already that the first four of Eqs. (14) will not be satisfied by the numerical values of Table VII we add to each equation a term denoted by  $\Delta$ , which we call the closure failure. Thus we have

$$\Omega C_{sr} = \frac{1}{2} (p-3) p W + \Delta(\Omega C), \quad \Omega dC_{sr}/d \ln r = -\frac{1}{2} (p^2 - 2p - 6) p W + \Delta(\Omega dC_{sr}/d \ln r), \quad (16)$$

$$\Omega C_{sr}' = \frac{1}{4} (p-7) p W + \Delta(\Omega C'), \quad \Omega dC_{sr}'/d \ln r = -\frac{1}{4} (p^2 - 6p - 14) p W + \Delta(\Omega dC_{sr}'/d \ln r).$$

In these equations the first term on the right results from substituting the exponential form  $W=A \exp(-pr/r_0)$  in each of Eqs. (14); it can be evaluated from the values of  $p$  and  $W$  shown in Table VIII. The closure failures have been computed from Eqs. (16) using Table VII, and are entered in Table VIII. They are also shown in Fig. 2 as fractions of the corresponding total experimental quantity.

It will be observed that the closure failures,  $\Delta$ , for the shear constants themselves are all negative (except for  $C'$  in copper), and range from small in copper through a large amount in silver to values in gold which are larger than the total experimental stiffnesses themselves. The closure failures of the hydrostatic strain derivatives are positive in sign, and increase rapidly again in the sequence copper, silver, gold but are substantial fractions of the experimental values even for copper. Except for the shear stiffnesses of copper, these closure terms are considerably larger than can be reasonably accounted for on the basis of experimental error or uncertainty in the theoretical long range

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