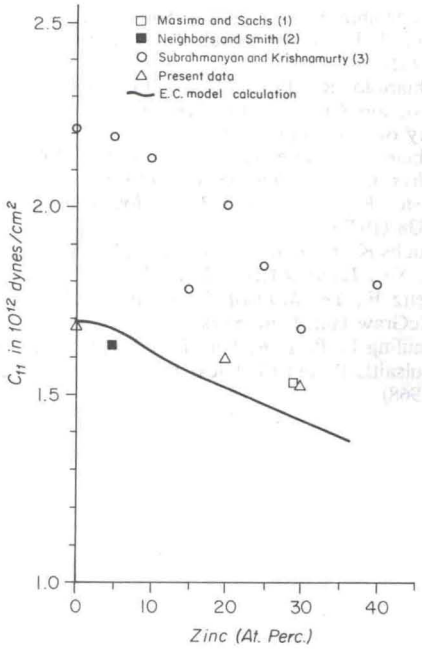

Fig. 3. Young's modulus as function of composition.

Table 1.

Alloy (Zn/Cu)	0·0/1·0	0·19/0·81	0·29/0·71
a (Å)	3·6147	3·658	3·681
C (10^{12}dyn/cm^2)	0·755	0·737	0·719
C' (10^{12}dyn/cm^2)	0·235	0·189	0·191
B_s (10^{12}dyn/cm^2)	1·374	$1·33_9$	$1·26_6$
B_T (10^{12}dyn/cm^2)	1·346	$1·29_2$	$1·21_8$
$\partial C/\partial P$	2·37	$2·3_7$	$2·4_9$
$\partial C'/\partial P$	0·592	$0·47_7$	$0·52_0$
$\partial B_s/\partial P$	5·84	$5·7_3$	$7·6_5$

$C = C_{44}$, $C' = 0·5\ (C_{11} - C_{12})$, $B_s = (C_{11} + 2C_{12})/3$

the equation of state of the noble metals [9] and the elastic and cohesive properties of Cu–Au alloys [8].

As is discussed in Ref. [9] the cohesive energy of the noble metals may be expressed in the form

$$\epsilon_{coh} = \frac{A}{r_s^3} + \frac{F}{r_s^2} + \frac{B}{r_s} + \epsilon_{corr} + 6\epsilon_p$$

where

$$\epsilon_p = D(-\alpha d) - Cd^6. \qquad (1b)$$

In the above equations A, F, B, D, α and C are characteristic constants determinable for each of the noble metals; r_s and d are the Wigner–Seitz cell radius and the interatomic distance, respectively, ϵ_{corr} the correlation energy and, ϵ_p the pairwise interaction energy.

The contributions to the shear constants can be separated, into the parts corresponding to electrostatic interactions and pairwise interactions (according to the Fuch's equations [10]) and a contribution from the distortion of the Fermi surface. The bulk modulus, on the other hand, is proportional to the second derivative of the cohesive energy with respect to volume.

The elastic constants for the Cu–Zn alloys were calculated on the basis of the following assumptions:

(a) The contributions to the elastic constants from electron cell and electrostatic interactions were calculated on the basis of an average electron density of $(1 + x_{Zn})$ electrons/cell with a corresponding average positive charge on each ion. It was assumed, as would correspond to a free electron model, that the electron cell constants A, B and G vary with $n^{1/3}$ and F with $n^{2/3}$, where n is the average number of conduction electrons/atom. (e.g. see Ref. [10]).

(b) The constants of the repulsive part of the pairwise potential were assumed to be the same as those for copper, since the configuration of the closed electron shells is likely to be very similar for the two ions.

(c) The Van der Waals interaction constant C for zinc was determined from polarizabilities estimated from Pauling's "Mole Refraction" constants [12], as has been done previously for the noble metals [13], ($C_{Cu} = 57·6$ kcal Å^6/gr. at, $C_{Zn} = 50·3$ kcal Å^6/gr. at.)

(d) The contribution from Fermi surface distortion to the shear moduli was assumed constant and equal to that determined (by difference between experimental and calculated values of shear moduli) for copper [9].

The elastic moduli so calculated are compared to the expermental values in Table 2, and the corresponding values of C_{11}, B_s and E (calculated by the Kneer equations) have been traced in Figs. 1–3. In view of the approximations made, the agreement of calculated and experimental data seems satisfactory. The excessive decrease of the calculated bulk modulus with composition possibly indicates that the approximation relative to the changes of the electron cell constants with composition is the least adequate. On the other hand, the better agreement of calculated and experimental shear moduli suggests that the Born–Mayer potential between zinc and copper atoms is not, in fact, very different from that between copper ions.

This is further support for a previously suggested conclusion [10] that the Born–Mayer potentials calculated from elastic and cohesive properties, after subtracting the

Table 2. Calculated and experimental elastic moduli (in 10^{12} dyn/cm^2)

Alloy (Zn/Cu):	0·05/0·95	0·10/0·90	0·19/0·81	0·29/0·71
C_{44}^P	0·848	0·810	0·754	0·692
C_{44}^e	0·292	0·315	0·361	0·414
C_{44}^f	−0·378	−0·378	−0·378	−0·378
C_{44} (calc)	0·762	0·747	0·737	0·728
C_{44} (exp)	0·742†		0·737	0·719
C'^p	0·248	0·238	0·222	0·205
C'^e	0·031	0·034	0·038	0·044
C'^f	−0·034	−0·034	−0·034	−0·034
C' (calc)	0·245	0·238	0·226	0·215
C' (exp)	0·221†		0·189	0·191
B_s (calc)	1·348	1·287	1·224	1·161
B_s (exp)	1·339†		1·339	1·266

†95·41%Cu–4·59%Zn. Ref. [2].

electron effects, may be physically more realistic, and applicable to a broader range of problems.

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