Erratum: Structural properties of ordered high-melting-temperature intermetallic alloys from first-principles total-energy calculations [Phys. Rev. B 41, 10 311 (1990)]

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A sentence fragment was inadvertently deleted from the last sentence on p. 10 316. The sentence should read as follows:

For cubic materials Fine *et al.* found that the data comparing melting temperatures and the equilibrium value of C_{ii} could be fitted by the straight line

$$T_m = 553\ \text{K} + (591\ \text{K/Mbar}) C_{11} \pm 300\ \text{K}\ , \tag{29}$$

while for tetragonal materials

$$T_m = 354\ \text{K} + (450\ \text{K/Mbar})[\tfrac{1}{3}(2C_{11} + C_{33})] \pm 300\ \text{K}\ . \tag{30}$$

A more serious error occurred in our calculation of the electronic structure of RuZr. An error in the interpolation of the muffin-tin part of the LAPW potential to the APW mesh gave the wrong band structure and density of states (DOS). We have corrected this error and recalculated the band structure and DOS for the $B2$ phase of RuZr. The results are displayed in the revised Figs. 9 and 10 shown here. The final paragraph on p. 10 320 should read as follows:

The energy bands of $B2$ RuZr are presented in Fig. 9. The main characteristic of this structure is the narrowness of the d Ru bands below the Fermi level. This feature is also shown in Fig. 10, where the RuZr DOS and its components are presented. Note the very high DOS with t_{2g} Ru symmetry below E_F and the low DOS at E_F. Table VII lists the E_F, the DOS at E_F, and the l components of the DOS at E_F.

We also present the correct Table VII.

These changes do not affect the main conclusion of the paper, the fact that the elastic moduli and equation of state of ordered intermetallic alloys can be quite accurately calculated from first-principles total-energy calculations.

TABLE VII. (a) Density of states at the Fermi level, and (b) l components of the DOS at E_F.

(a)

	E_F	DOS
SbY	0.383 40	6.099 84
CoAl	0.822 79	8.109 00
RuZr	0.785	7.304 32
NbIr	0.835 95	21.44

(b)

Crystal	Site	s	p	e_g	t_{2g}	f
SbY	Sb	0.009 98	1.843 95	0.018 19	0.241 83	0.011 71
	Y	0.021 23	0.115 09	0.216 59	1.413 72	0.066 10
CoAl	Co	0.096 35	0.500 57	5.181 81	0.936 17	0.009 81
	Al	0.014 85	0.420 95	0.006 54	0.177 73	0.005 51
RuZr	Ru	0.080 15	0.560 55	1.821 19	0.891 21	0.102 64
	Zr	0.052 00	0.359 22	1.635 98	0.215 14	0.063 44
				d		
NbIr	Nb	0.1686	0.5948	8.718		0.1527
	Ir	0.0806	0.8058	5.405		0.0648

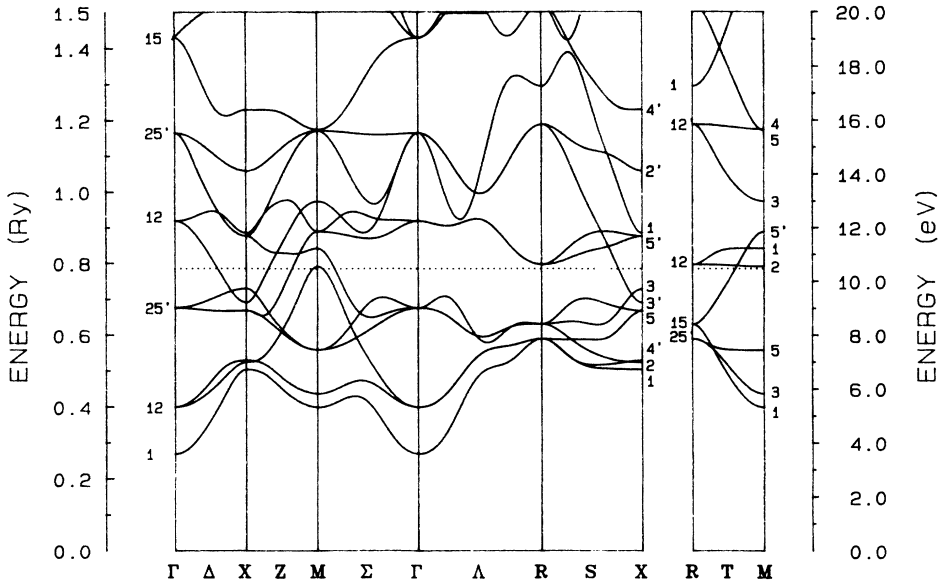

FIG. 9. Band structure along the high-symmetry directions of the $B2$ phase of RuZr at the lattice constant $a = 3.22$ Å, using the APW method to do the calculations. The dashed horizontal line shows the location of the Fermi level.

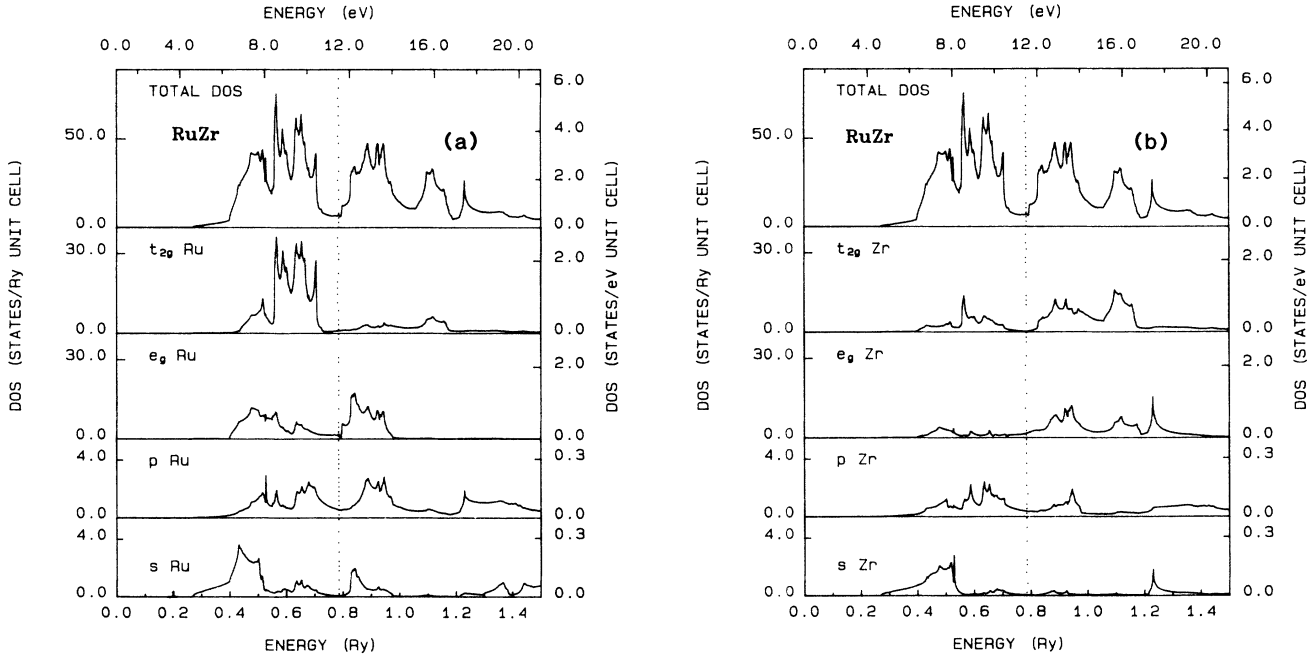

FIG. 10. Density of states of the $B2$ phase of RuZr at the lattice constant $a = 3.22$ Å, calculated via the APW method. The top plot shows the density of states, while the lower graphs show the symmetry-decomposed partial density of states on each site. The Fermi energy is marked by the dotted vertical line. Note the different scales in the various components of the DOS. (a) The total DOS and the partial DOS at the Ru site. (b) The total DOS and the partial DOS at the Zr site.