*Journal of Alloys and Compounds, 211/212* (1994) 522–524
*JALCOM 092*

# Zener relaxation strength in b.c.c. and f.c.c. alloys

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## Abstract

Welch and Le Claire's theory (*Philos. Mag., 16* (1967) 981) is extended to include the relaxation strength of the Young and bulk moduli. A complete set of equations is given for the calculation of the relaxation strength of all the moduli in both f.c.c. and b.c.c. alloys. The relaxation strength of the Young modulus in $\beta$-brass and $Cu_3Au$ is discussed in terms of these equations. Some ordering parameters are obtained from the anelastic data, which are confirmed by independent estimates.

## 1. Theoretical background

Recently Povolo and Mosca [1] have extended Welch and Le Claire's theory [2] to the case of longitudinal excitations, where the relaxation of the Young modulus is involved. Not only f.c.c. but also b.c.c. lattices were considered to obtain a complete set of equations describing the Zener relaxation strength of the torsion, Young and bulk moduli in substitutional alloys of cubic structure. This approach takes into account both first- and second-nearest-neighbour interactions and order parameters out to eight neighbours.

The complete set of equations obtained is

$$\Delta_{S''}=\Delta_K=-\frac{2m_Am_B}{K_r\Omega}\frac{a_0^2}{3}\frac{1}{V_1}\left(\frac{dV_1}{dr}\right)^2 \times\left(\eta_1^1+\frac{1}{2^{1/2}}(2\eta_1^2+\eta_2^1)R+\eta_2^2R^2\right) \tag{1}$$

for f.c.c.

$$\Delta_{S''}=\Delta_K=-\frac{2m_Am_B}{K_r\Omega}\frac{a_0^2}{3}\frac{1}{V_1}\left(\frac{dV_1}{dr}\right)^2 \times\left(\eta_1^1+\frac{3^{1/2}}{6}(4\eta_1^2+3\eta_2^1)R+\eta_2^2R^2\right) \tag{2}$$

for b.c.c.

$$\Delta_S=\Delta_C=-\frac{2m_Am_B}{\Omega C_r}\frac{a_0^2}{V_1}\left(\frac{dV_1}{dr}\right)^2\frac{\zeta_1^1}{3} =-\frac{2m_Am_BS_r}{\Omega}\frac{a_0^2}{V_1}\left(\frac{dV_1}{dr}\right)^2\frac{\zeta_1^1}{3}\quad\text{for b.c.c.} \tag{3}$$

$$\Delta_{S'}=\Delta_{C'}=-\frac{m_Am_B}{\Omega C_r'}\frac{a_0^2}{V_1}\left(\frac{dV_2}{dr}\right)^2\zeta_2^2 =-\frac{m_Am_BS_r'}{\Omega}\frac{a_0^2}{V_1}\left(\frac{dV_2}{dr}\right)^2\zeta_2^2\quad\text{for b.c.c.} \tag{4}$$

where $a_0$ is the lattice parameter, $m_A$ and $m_B$ are the atomic fractions of A and B atoms respectively in the alloy, $\Omega$ is the atomic volume, $dV_1/dr$ is the gradient of the ordering energy at the nearest-neighbour (NN) separation, $R$ is the ratio of the gradient at the next-nearest-neighbour (NNN) separation to that at the NN separation, *i.e.* $R=(dV_2/dr)/(dV_1/dr)$, $S_r$ is the relaxed compliance for a (001)[010] shear, $S_r'$ is the relaxed compliance for a (110)[1$\bar{1}$0] shear, $S_r''$ is the relaxed compliance for a hydrostatic pressure, $V_1$ and $V_2$ are the ordering energies for NN and NNN atoms respectively and $r$ is the interatomic distance. The coefficients $\eta$ and $\zeta$ are functions of temperature and represent coupling constants which couple stress-induced changes in the ordering energy to changes in the degree of order.

The anisotropy of the relaxation can be characterized in terms of the "anisotropy factor" $A$ defined as [2]

$$A=\frac{S_r\Delta_{S'}}{S_r'\Delta_S} \tag{5}$$

Taking into account eqns. (3) and (4), eqn. (5) can be written as

$$A=\frac{3}{2}\frac{\zeta_2^2}{\zeta_1^1}R^2\quad\text{for b.c.c.} \tag{6}$$

0925-8388/94/$07.00
*SSDI* 0925-8388(93)00092-D

Figure 1 shows the dependence of the anisotropy factor for b.c.c. alloys of compositions AB and $A_3B$ on the reduced temperature and gradient ratio using $\rho = V_2/V_1 = 0.5$ [3]. The temperature dependence of $A$ comes from the fact that the coupling constants are temperature dependent.

The Young and torsion moduli can be calculated by combining $\Delta_S$, $\Delta_{S'}$ and $\Delta_{S''}$ with the orientation $\Gamma$ of the crystal relative to the stress axis. In fact, for the relaxation strength of the Young modulus the following expression can be written:

$$\Delta_E = \frac{(\delta S' + \delta S'') - 3(\delta S' - \delta S)\Gamma}{(S'_u + S''_u) - 3(S'_u - S_u)\Gamma} \tag{7}$$

It is generally observed that the temperature dependence of the relaxation strength obeys a Curie–Weiss-type law [4]

$$\Delta_M^{-1} \propto T - T_M^{\mathrm{ANE}} \tag{8}$$

where $T_M^{\mathrm{ANE}}$ is the anelastic critical temperature at which ordering would occur spontaneously if atomic movements were possible. With eqns. (1)–(4) $T_M^{\mathrm{ANE}}$ can be expressed analytically only in the high temperature limit where the short-range order parameters $\alpha_i$ are lower than unity and for $R = 0$. In general the exact temperature dependence of the relaxation strength can be evaluated only numerically. For example, Fig. 2 shows the values obtained for the temperature dependence of $\Delta_S^{-1}$ and $\Delta_{S'}^{-1}$ for b.c.c. alloys with composition $A_3B$. It is evident that $\Delta_S^{-1}$ and $\Delta_{S'}^{-1}$ change linearly with $T$ up to high values of the reduced temperature ($kT/2V_1$).

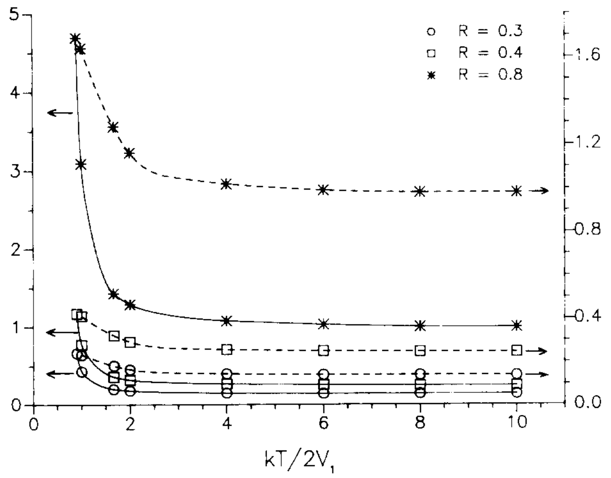

Fig. 1. Anisotropy factor *vs.* reduced temperature for b.c.c. alloys of compositions $A_3B$ (full curve) and AB (dashed curve) with $\rho = 0.5$.

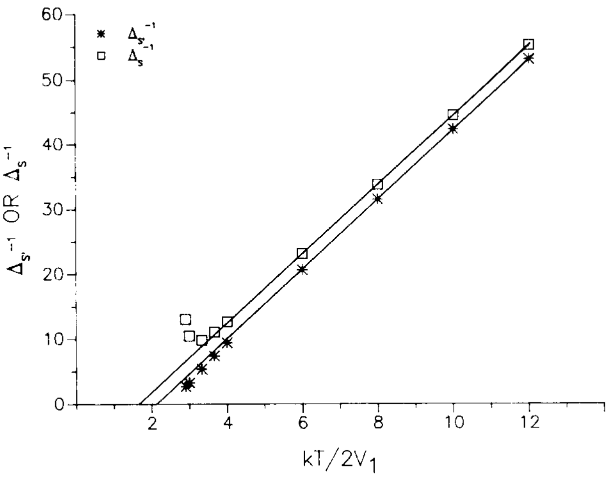

Fig. 2. Reciprocal of relaxation strength (arbitrary units) of $S$ and $S'$ shear *vs.* reduced temperature in b.c.c. alloys of composition $A_3B$. The straight lines give the high temperature limit.

## 2. Applications

Expressions (1)–(4) and those obtained for $\Delta_S$ and $\Delta_{S'}$ in f.c.c. alloys by Welch and Le Claire [2] can be used to deduce the relaxation strength of the Young modulus in f.c.c. and b.c.c. alloys.

A re-evaluation of the experimental results of Artman and Thompson [5, 6] on b.c.c. β-Cu–50at.%Zn alloy gives the following values: $\Delta_S = 4 \times 10^{-4}$ and $\Delta_{S'} = 15.4 \times 10^{-4}$ at 588 K. These values were computed by assuming a negligible contribution from $\delta S''$, which should be very small owing to the small value of $S''$ itself [6].

Murakami *et al.* [7] reported a value $V_1 = 184$ K for β-CuZn, obtained by reproducing the phase diagram of $Ag_xCu_{53-x}Zn_{47}$ alloys, which leads to a reduced temperature of 1.59.

The anisotropy factor for this alloy is 0.4, which gives $R = \pm 0.43$ according to eqn. (5) and coupling constants obtained by interpolating between the values reported by Povolo and Mosca [1]. Then, by using eqn. (4), it is possible to calculate $dV_1/dr$ as $\pm 2.25 \times 10^{-11}$ N. Once $R$ and $dV_1/dr$ are known, $\Delta_{S''}$ and $\Delta_E$ can be evaluated. A positive value for $R$, *i.e.* $R = 0.43$, was chosen, since this leads to a better agreement with the experimental data reported by Artman and Thompson for $\Delta_E$ (see Fig. 3).

Figure 4 shows $T_E^{\mathrm{ANE}}$ obtained theoretically *vs.* $\Gamma$. It is clear that $T_E^{\mathrm{ANE}}$ is strongly anisotropic. Unfortunately, there are no experimental values for these temperatures.

More recently Povolo and Armas [8] reported anelastic data in f.c.c. $Cu_3Au$ at 673 K where $\Delta_{S''}$ is smaller than $\Delta_{S'}$. Then a first approximation for $R_E$ can be written in the simple form

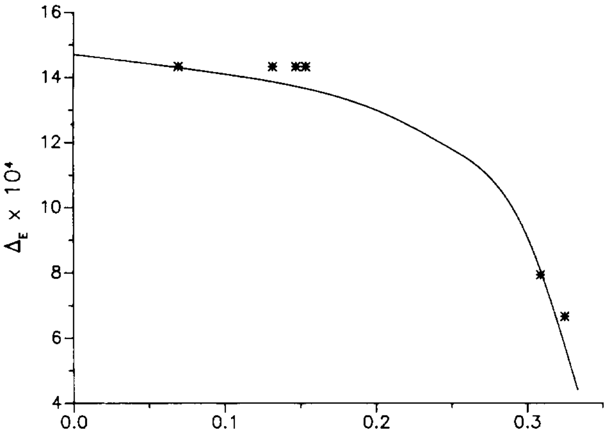

Fig. 3. Orientation dependence of relaxation strength of Young modulus in $\beta$-brass: *, values calculated from refs. 5 and 6; curve, theoretical calculations.

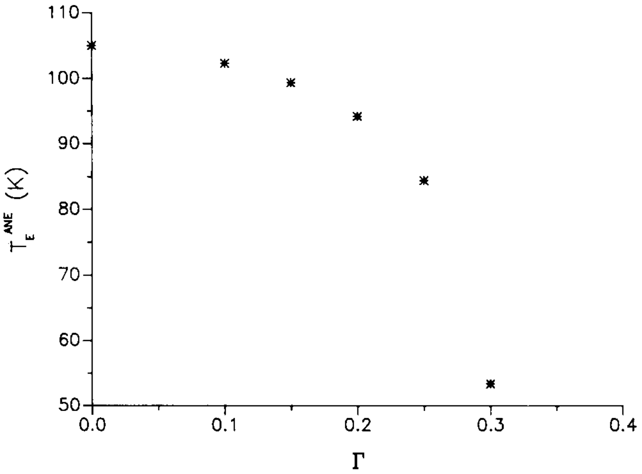

Fig. 4. Theoretical orientation dependence of anelastic critical temperature for Young modulus in $\beta$-brass.

$$R_E = \frac{\Delta_{E\langle 100\rangle}}{\Delta_{E\langle 111\rangle}} \approx \frac{\Delta_{S'}}{\Delta_S} = 8.61$$

The value $R_E = 8.01$ is obtained theoretically by using $V_1 = 358$ K, $R = -0.25$ and $dV_1/dr = -1.25 \times 10^{-9}$ N as reported in ref. 9. It is seen that the theoretical value is very close to the experimental one.

## 3. Discussion

Some ordering parameters have been obtained in a $\beta$-CuZn alloy by analysing the orientation dependence of the Zener relaxation and assuming $R > 0$, $\rho > 0$ and $V_1 > 0$. The value used for $R$ can be confirmed by independent calculations. In fact, de Rooy *et al.* [10] estimated the ordering energy as a function of the interatomic separation (by pseudopotential theory) for the CuZn system. From Fig. 3 of ref. 10 it is clear that $dV_1/dr$ and $dV_2/dr$ have the same sign, so that $R > 0$ ($R \approx 0.48$), as was assumed in the interpretation of the anelastic data. Harrison and Paskin [11] have provided theoretical reasons for expecting that long-range oscillatory interactions should be significant in the $\beta$-CuZn system, *i.e.* $V(r) \propto \cos(2k_f r + \phi)/r^3$, where $k_f$ is the Fermi momentum and $r$ is the interatomic separation. In addition, these authors suggest that the most appropriate values for CuZn are $\phi = \pi/2$ and $\pi/2 - 0.28$. Then with $\phi = \pi/2$ we find $R = 0.30$, which is in agreement with the value obtained from the anelastic data.

The values of $R$ and $dV_1/dr$ obtained by Povolo and Armas in $Cu_3Au$ alloys (through anelastic data) have also been confirmed by independent estimates.

## 4. Conclusions

The sets of equations given by Welch and Le Claire and by Povolo and Mosca can be used to describe the main aspects of the relaxation strength of the Zener relaxation in f.c.c. and b.c.c. alloys.

The ordering parameters obtained from the anelastic data can be confirmed by independent estimates.

More experimental work on the orientation, temperature and composition dependence of the relaxation strength is needed to confirm the results reported in this paper.

## Acknowledgments

This work was supported partially by the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) and the "Proyecto Multinacional de Investigación y Desarrollo en Materiales" OAS-CNEA.

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