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Fitting of experimental data to the Granato-Lücke model

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A new, direct and more accurate method than the usual Granato–Lücke plot is given, for the fitting of the experimental data to the theory. Some results reported in the literature are analysed and it is shown that all the aspects of the theory must be taken into account in order to obtain meaningful results for the several dislocation parameters.

1. Introduction

The Granato–Lücke model [1] for the amplitude-dependent damping produced by the unpinning of dislocations from impurity atoms has been widely used to obtain information on dislocation–solute atoms interactions and on the properties of dislocations. Although this is a zero-temperature model, it was used, with apparent success, to obtain values of dislocation parameters from damping data measured at high temperatures.

Bauer and co-workers [2, 3] among others have used the so-called Granato–Lücke plot to obtain values for the binding free energies between solute atoms and dislocations in several alloys. More recently, the same plot has been used by Atrens [4] to obtain the binding energy between oxygen atoms and dislocations in Zr–O alloys, and by Burdett and Wendler [5] for solute atoms and dislocations in zinc. Povolo [6] has recently commented on the validity of the dislocation parameters obtained from the Granato–Lücke plots and on those calculated from the temperature dependence of the slopes of those plots. These comments have led to a controversial discussion [7, 8] and it is not clear when a set of experimental damping data can really be described by the Granato–Lücke model.

A new method of fitting the experimental data to the theory will be given that does not rely on the linearity of the Granato–Lücke plots and the results are compared directly and unambiguously with the theoretical expressions.

2. Results and discussion

The amplitude-dependent damping, Δ_H, due to the unpinning of dislocations including strain distributions in the specimens, is given by [9]

$$\Delta_H = C_1(C_2/\epsilon_0)F(C_2/\epsilon_0)\exp(C_2/\epsilon_0), \quad (1)$$

where ϵ_0 is the strain amplitude, C_1 and C_2 are constants for a particular dislocation–point defect configuration and $F(C_2/\epsilon_0)$ is a function that takes into account the strain distribution in the specimen.

A plot of equation 1 as $\log \Delta_H \epsilon_0$ versus $1/\epsilon_0$ (Granato–Lücke plot) at small strains gives a straight line of slope C_2. This is the plot generally used in the literature and the binding energy between dislocations and impurity atoms is obtained from the temperature dependence of C_2 [6]. In general, no attention has been given to the parameter C_1.

The experimental data can be fitted to the theory in a more direct way by plotting the logarithm of the normalized damping Δ_H/C_1, versus the logarithm of the normalized strain, ϵ_0/C_2, given by Equation 1. Such a plot is shown in Fig. 1 for longitudinal (Δ_l/C_1) and torsional (Δ_t/C_1) excitations. The approximate limit in the strain amplitude $(\epsilon_0/C_2 \leqslant 0.25)$ imposed by the model [1] is shown in the same figure.

The experimental damping versus strain data, (Δ_H, ϵ_0) can be compared with Fig. 1 and Equation 1 by plotting them as $\log \Delta_H$ versus $\log \epsilon_0$ with the same scales as for Fig. 1. By translation, these

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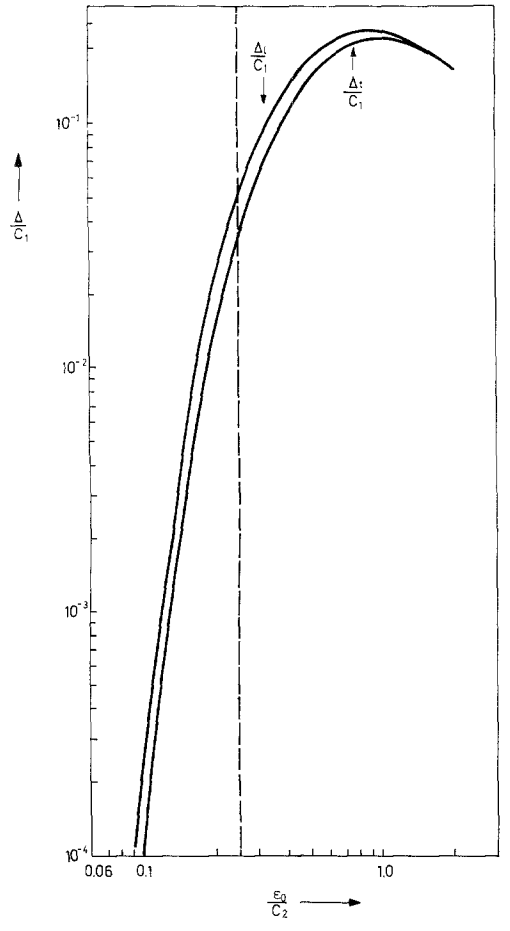

Figure 1 Logarithmic plot of Equation 1 for torsional and longitudinal excitations.

curves can be superimposed on part of the theoretical curve, and C_2 can be obtained from the coincidence of some value of ϵ_0 from the experimental curve with a ϵ_0/C_2 value of the theoretical curve, and C_1 from that of an experimental damping value with the corresponding theoretical Δ_H/C_1 value.

To illustrate the procedure, some published data which have previously been analysed using the Granato–Lücke plot [6] will be fitted to Equation 1 in the way suggested above.

Atrens' [4] data for Zr–O alloys obtained in torsion and, Oren *et al.*'s [3] results for Cu–Si alloys obtained in longitudinal excitations, are shown in Figs. 2 and 3, respectively. The points indicate the experimental data and the curves the part of the corresponding theoretical curve of Fig. 1 where the fitting was made. It is seen that there is only one way to fit the data to Equation 1, and no straight lines have to be drawn through the experimental points, in some cases rather subjectively, as for the case of the Granato–Lücke plot.

The ϵ_0/C_2 and Δ_H/C_1 theoretical values chosen to calculate C_1 and C_2 are marked on each curve and the values obtained for these parameters are shown in the same figures as a function of the reciprocal of the absolute temperature.

The C_2 values are quite similar to those reported by Atrens and Richtie [7] and Oren *et al.* [3]. As shown in both figures, C_2 does not increase linearly with $1/T$ as assumed by Atrens [4] and Oren *et al.* [3]. Furthermore, Atrens [4] and Atrens and Richtie [7] only considered the high temperature data of Fig. 2, drawing the average straight line shown in the figure, and obtaining a binding energy, U_B, of the order of 0.2 eV.

Oren *et al.* [3] used the average straight line at high temperatures shown in Fig. 3 to calculate the binding energy, obtaining a value of ~0.5 eV (or ~0.25 eV by using a factor of 2 in the expression for the concentration of solute atoms at the dislocation core [3]). It is seen that both values are meaningless since if one chooses the low temperature data of Figs. 2 and 3, where the Granato–Lücke theory should be more applicable, C_2 would be practically constant with temperature in Fig. 2, and a binding energy of the order of 0.09 eV would be obtained from Fig. 3.

These incongruities arise from the fact that only partial aspects of the theory were considered by these authors and a more detailed analysis of the experimental data shows that they are not described by the Granato–Lücke model. In fact, C_1 and C_2 are proportional to $1/L_c$ [6], where L_c is the average distance between minor pinning points, so that both parameters should show the same temperature dependence. As shown in Figs. 2 and 3 this is not the case, and in the region considered by Atrens [4], C_1 even decreases with $1/T$. Furthermore, $C_1 = \Omega\Delta_0\Lambda L_N^3/\pi L_c$ [1], and assuming $\Lambda L_N^3 = 3$ (isotropic network), $\Omega = 1/25$ and $C = 1/2Gb^2$ results in

$$L_N/L_c \simeq 154 C_1 . \qquad (2)$$

Equation 2 gives the number of pinning points per major loop. Values between 0.047 and 0.23 are obtained for the number of pinning points by applying Equation 2 to the data of Fig. 2. Even if this equation gives only a rough estimate, it is seen that such values are meaningless. The situation is better for the data of Fig. 3 from which a value

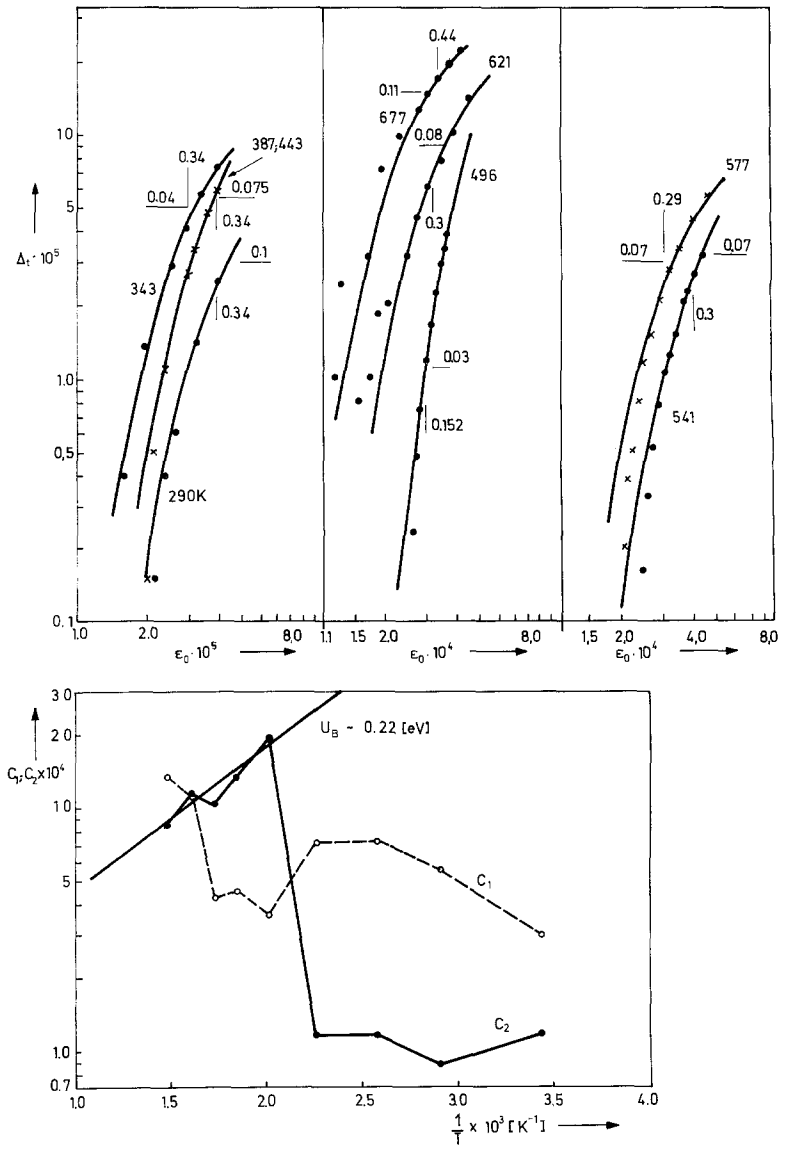

Figure 2 Fitting of the data of Figs. 1 and 2 of [4] to Equation 1.

of 9 is obtained, but the temperature dependence is not correct.

In conclusion, it is seen that even if the individual damping curves may be described by Equation 1 (which any function can be, at least in parts) and C_2 gives an Arrhenius plot (this is not the case for the data analysed) this is not enough to assert that the data are described by the Granato–Lücke model and the overall analysis of C_1 and C_2 must be considered. In addition, for the data just shown, the fitting was done at too high values of ϵ_0/C_2, i.e. beyond the limits imposed by the model.

From the arguments given above, it follows that the values obtained for the binding energies from the data of Figs. 2 and 3, are meaningless in the context of the Granato–Lücke model and it is unreasonable to estimate errors, as suggested by Fiore and Bauer [8]. It must be pointed out that similar inconsistencies were found [10] for the data reported by Burdett and Wendler [5] which were interpreted by the authors using the Granato–Lücke plot.

Finally, Fernandez and Povolo [11] have interpreted their amplitude-dependent damping and modulus defect data in zirconium and zircaloy-4

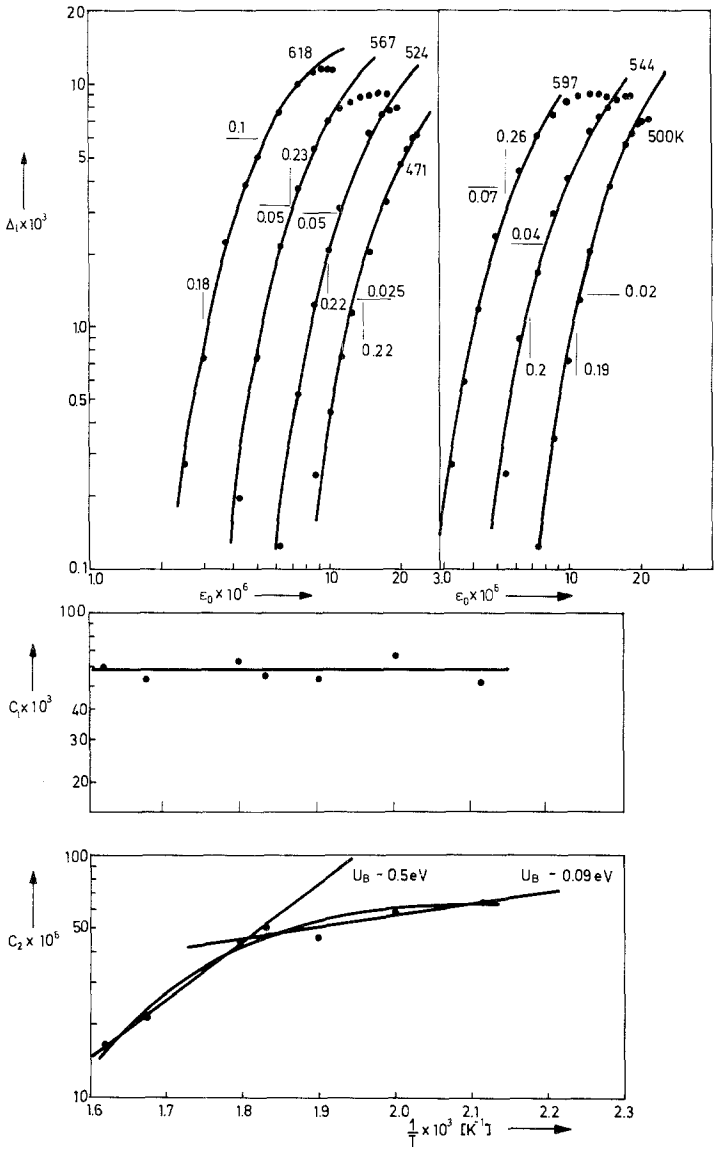

Figure 3 Fitting of the data of Fig. 1 of [3] to Equation 1.

in terms of an interaction between extended dislocation and oxygen atoms by using a different approach. A theory given by Blair *et al.* [12], which takes thermal activation into account, was used and a value of 1.2 eV was obtained for the binding energy, and not 0.18 eV as given by Atrens [4] and Atrens and Richtie [7].

3. Conclusions

A model has been proposed for fitting experimental data to the Granato–Lücke model in an unambiguous way. Unfortunately, the typical data just analysed are not described quantitatively by the model, especially in the generally assumed temperature dependence of C_1 and C_2. This was found to be the case with other data, even with those originally analysed by Granato and Lücke [13], so that it may be said that a numerical confirmation of the model, at least in the predicted temperature dependence of the parameters C_1 and C_2, has not yet been established.

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