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DISCUSSION :
POINT DEFECTS - DISCUSSION AND GENERAL REMARKS

M. WELLER

*Max-Planck-Institut für Metallforschung, Institut für
Werkstoffwissenschaften, D-7000 Stuttgart, F.R.G.*

Point defects, that is defects of atomic size, in crystalline solids may give rise to Snoek type relaxations, if they are elastically anisotropic, i.e. if their symmetry is lower than that of the crystal. Application of an elastic stress leads to an orientational redistribution of the elastic dipoles. With the assumption that Boltzmann statistics may be applied for this redistribution, and that the reorientation jumps are thermally activated the following equations hold for the relaxation strength, Λ , and for the relaxation time, τ :

$$\Lambda \propto 1/kT \cdot c (\delta\lambda)^2, \quad \tau^{-1} = \tau_{\infty}^{-1} \exp(H/kT) \quad (1a,b)$$

(c = concentration of dipoles, $\delta\lambda$ = anelastic shape factor, H = activation enthalpy for reorientation; the preexponential factor, τ_{∞} is about 10^{-14} s). In alternating stress fields (internal friction experiments) the well known Debye equation for energy absorption,

$$Q^{-1} = \Lambda \omega\tau / (1 + \omega^2\tau^2), \quad (2)$$

results from this approach ($\omega = 2\pi f$ = measuring frequency).

Measurements of Snoek type relaxations described by equations (1,2) have been successfully applied in the past decades - since its discovery in 1941 - to study the properties of heavy interstitial foreign atoms (IFA) such as O, N, C in b.c.c. metals (diffusion, precipitation, interstitial concentration) if their reorientation is combined with a diffusional jump, defects in irradiated metals (mainly self interstitial atoms, and their agglomerates and complexes with solute atoms), or defects in non-metallic crystals. Fig. 1 shows schematically simplified for a monatomic crystal possible defect configurations which may cause Snoek type relaxations (see legend).

The state of knowledge at the end of the seventies is excellently presented in two books /1,2/ and several review articles in conference proceedings /3/. Not many open questions seemed to remain.

At that time the situation changed partially for several reasons. There was considerable progress in the preparation of very pure samples. Measuring techniques were improved by application of electronic components and computers. Furthermore, theories for interpretation of experiments were developed (and refined) considerably. As a result, some problems which were considered to be undisputably solved came into discussion again.

Another development which may be observed for some time in this field is the tendency to study advanced materials with more complicated defect structures.

The contributions to this conference brought examples for both developments:

One example is the controversy on the effect of interaction between IFA in b.c.c. metals at high solute contents. This discussion (see also ICIFUAS-7 (1981) and ICIFUAS-8 (1985)) was continued at his conference. The clustering model /4/ predicted (and claimed to show) that clusters of two, three or more IFA (pairs, triplets etc.) should be formed by (attractive) interaction and cause additional Debye peaks. This model was /5/ and still is doubted /6/ since very precise and detailed internal friction measurements do not allow decomposition of the Snoek peaks in con-

concentrated alloys into several relaxation peaks (discrete values of τ) but rather indicate a continuous broadening of the peak (continuous distribution of τ). Precise measurements of the relaxation parameters and their variation with concentration were presented at the present conference. Problems arising from modulus measurements (which should show indeed a corresponding behaviour) and from background subtraction in internal friction curves were discussed. A physical model to explain the continuous broadening (distribution in τ) based on long range interaction of IFA is not available at the moment and has to be developed.

As concerns the second development a series of papers is concerned with more complicated materials. One group at this conference deals with the properties of heavy IFA in technical alloys such as Zr-based b.c.c. alloys /7/ or ferritic steels /8/. Another group studies atomic defects in non-metallic solids (ceria, quartz, vanadate glasses). For Sc-doped CeO₂ /9/ internal friction measurements were combined with dielectric thus allowing study of the same defects as elastic and electric dipoles. A relaxation peak at higher temperatures is assigned to a defect complex consisting of a Sc ion and an oxygen ion vacancy. A peak at lower temperatures is correlated with the anelastic relaxation of Sc-ions - which are considerably smaller than the Ce-ions - by assuming that they are in an off-center position. This is an example of an anisotropic defect formed by isolated foreign atoms. (ions). These are usually, as demonstrated in Fig. 1 for the simplified case of a monatomic crystal, expected to behave isotropically. A possible physical reason for the off-center position in ceria was discussed. Apparently an asymmetric cage is formed by movements of the 8 surrounding oxygen ions. Electronic effects (as e.g. for the Jahn Teller effect) do not play a role. Relaxation peaks occurring in vanadate glasses (with τ_{∞} -values between 10⁻⁵ and 10⁻⁹ s) are interpreted by a polaron hopping /10/ mechanism.

A considerable number of papers at the present conference dealt with hydrogen in metals.

Hydrogen makes an exception as an atomic defect since for isolated H atoms - in contrast to the heavy IFA - no Snoek effect is known in b.c.c. metals. This is almost certainly due to the smallness of the elastic dipole moment $\delta\lambda$ (eq. 1) (in addition the solubility in some metals is rather low). Thus hydrogen in cubic metals is studied by indirect methods. In concentrated alloys short range ordering of H in pairs (Zener effect of solute pairs, see Fig. 1) is observed. For the Pd/Pt H system a relaxation strength $\Delta \propto (T-T_c)^{-1}$ was discussed /11/, i.e. it deviates from that expected for an ideal Snoek type relaxation ($\Delta \propto T^{-1}$, eq. (1a)).

The behaviour of hydrogen (deuterium) trapped by oxygen in Nb and Ta was studied both experimentally /12/ and theoretically /13/. Relaxation peaks occurring at about 4K are explained with a model which assumes that hydrogen is trapped near oxygen in an asymmetric double well potential. Transitions between the two positions - which correspond to different atomic configurations - occur by tunneling through the barrier. This is different from classical hopping over a potential barrier (by thermally activated jumps) as for Snoek type relaxations (eq. 1b). Theoretical calculations of the tunneling transitions, which may be phonon or electron assisted, and of the temperature variation of $\Delta(T)$ and $\tau(T)$ - which is different from eqs. (1a, b) - were compared with experimental results. Two points were extensively discussed. (i) The influence of the asymmetry of the double well potential on the tunneling transition. (ii) The possibility of distinguishing between phonon and electron assisted tunneling from the temperature dependence of the relaxation time. Apparently this is difficult since both give comparably good fits to the experiments. Altogether the examination of hydrogen relaxations at low temperature appears as a promising field for both experiments and further developments of theory.

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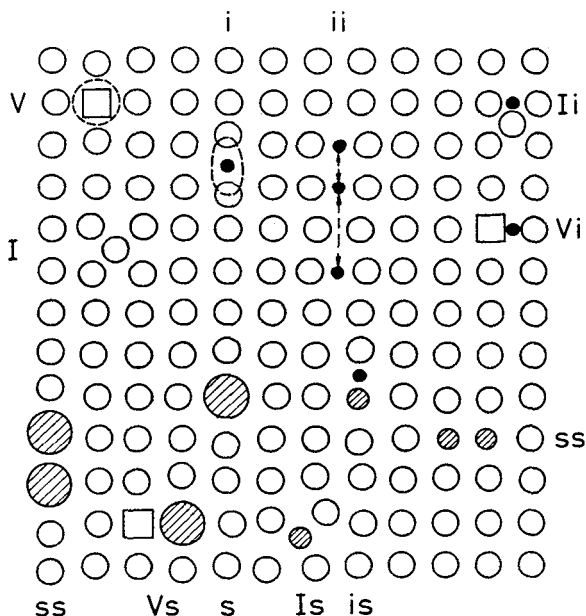


Fig. 1:

Configurations of atomic defects for a monatomic crystal (schematically).

V = vacancy, I = self interstitial atom, i = interstitial foreign atom (IFA),
s = substitutional foreign atom.

Isolated V and s defects are expected to be isotropic if they are not in an off-center position.

Interstitial atoms (I,i) may form elastic dipoles: In f.c.c. and b.c.c. metals self interstitial atoms (I) may be arranged as dumbbells. In b.c.c. metals interstitial foreign atoms (i) represent elastic dipoles causing the "classical" Snoek effect (in f.c.c. metals their distortion is isotropic). The isotropic and anisotropic distortions around a vacancy and an IFA are shown schematically.

More complicated anisotropic defects may be formed by ss, ii, or is-agglomerates or complexes of intrinsic defects (V,I) with foreign atoms (i,s) e.g. Vi, Ii, Vs, Is. Dotted lines between IFA should indicate their short and long range interaction.