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ANISOTROPIC THERMAL EFFECT ON Cd SINGLE CRYSTALS

E. DARTYGE and A. SADOC

LURE (CNRS, CEA, MEN), Bât. 209 D, F-91405 Orsay Cedex, France

Résumé : L'effet de l'agitation thermique sur les spectres EXAFS du cadmium est étudié pour 2 orientations différentes de monocristaux et en fonction de la température. Les déplacements moyens sont évalués pour les premiers voisins à l'intérieur du plan hexagonal et hors du plan hexagonal.

Abstract : The thermal motion is evaluated for oriented Cd single crystals, and for the first shells of distances. A separate evaluation is given for the 6 atoms out of the basal plane and for the 6 atoms inside the hexagonal plane.

I - Introduction

When studuying the lattice distorsion around Zn Cu alloys (1) we recorded the EXAFS spectra of pure Zn single crystals at various temperatures from 300 to 60 K in order to extract Zn phase shifts. Two orientations were chosen, the hexagonal c axis parallel to the polarisation vector e of the x ray beam and the a // e orientation. Even at 60 K, the contribution of the thermal motion seemed important for the c // e spectra since their amplitude was smaller by approximatly a factor of two of what should be expected for the 6 Zn atoms located out of the hexagonal plane.(this was not true for the a // e spectra) However, an analysis of the thermal motion versus temperature in this direction was not possible because the crystals did not support lower temperature than 60 k without breaking. We report here such an EXAFS study on cd oriented single Cd crystals which support temperatures varying from 30 to 300 K without any problem. Cd crystals have a h.c.p. structure with a c/a ratio = 1.886 at room temperature, which implies a large difference from a close packing of Cd atoms. In fact, at room temperature the first shell of 12 Cd atoms around the central atom consists of 6 Cd at 3.29A (out from the hexagonal plane) and 6 Cd at 2.98A (in the hexagonal plane). This difference from an ideal hcp structure is greater than in the case of Zn crystals which were studied by Brown et al (1). Therefore, the anisotropy of the thermal motion is expected to be more important in cadmium than in zinc as was shown by Thulke and Rabe (3) on polycristalline Cd : at 77 k they observed only the Cd-Cd distance characteristic of the 6 Cd in the hexagonal plane. The absence of a contribution of the off-plane atoms was explained by a large damping effect due to thermal motion. In fact, one of us (4) has also remarked that although the zeros of the polycristalline Cd at room temperature are characteristic of only the short distance, the amplitude in the

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100-200 eV range cannot be well fitted using only the 6 Cd-Cd pairs at 2.98 A : the second distance had to be taken into account. So the contribution of the Cd-Cd pairs at 3.29 A is not completely negligible, even at room temperature. However, as was pointed out by Thulke and Rabe, it is necessary to do the measurements on oriented single crystals in order to measure separately the thermal motion for these two different distances.

II - Sample preparation and experiment

The bulk cadmium single crystals were prepared by J.Godard (5). They were grown with a Bridgemann method, Laue orientated, cut at ~ 0.1 mm thick and then etched to obtain a platelet of ~ 25 µ. Two orientations were chosen : one class of crystals had the a and e axes parallel to the surface of the platelet ((01$\bar{1}$0) planes) and the other was cut perpendicular to the c axis, parallel to the hexagonal plane (0001). The platelets were put inside a cryostat, perpendicular to the x ray beam.

According to Beni and Platzmann (6) and considering the hexagonal structure of zinc, c//e EXAFS spectra give an estimation of absolute mean square displacement of the 6 Cd out of the basal hexagonal plane only, and a//e spectra, of the 6 hexagonal atoms with a small contribution of the off plane atoms. The spectra were recorded from 300 K to 30 K at DCI with a channel cut Si (400) monochromator which gives a resolution of about 15 eV at the Cd edge (26.7 keV). The EXAFS spectra were obtained after substracting a background constructed by smoothing the absorption spectra.

III - Results and discussion

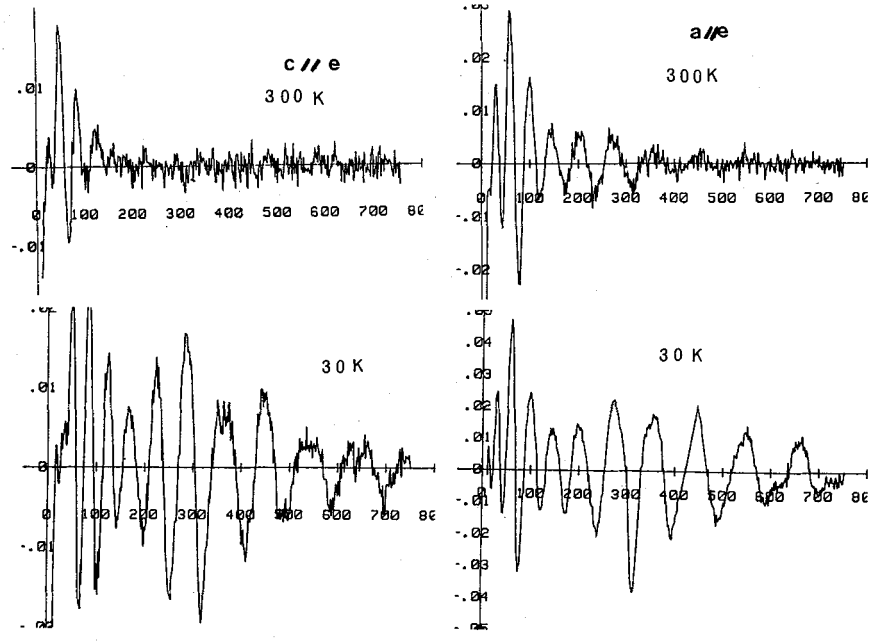


fig.1

Fig 1 shows the EXAFS spectra for both orientations, Fig 2 their Fourier transforms (FT). It can be seen that the amplitude of the c//e spectra is lower by a 2 factor than the a//e, even at 30 k. This can also be observed for the FT obtained in the same conditions for the two orientations. This amplitude comparison is made for the crystal parallel to (0 110) planes. The FT consist mainly of one peak (2.5-3.5A). Besides a bump towards low distances due to the structure of Cd backscattering amplitude, a small peak appears at 70 K towards large distances for a//e orientation, due to the contribution of the 6 off plane Cd atoms.

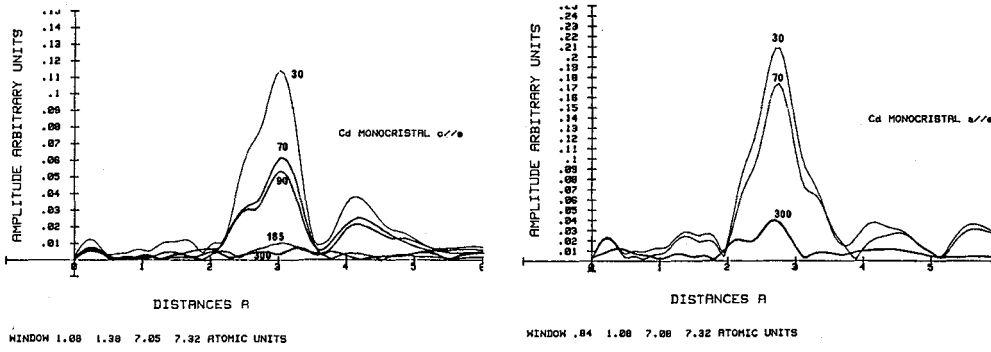


fig 2

In order to evaluate the thermal mean square displacement $\sigma//$ and $\sigma_\perp$ ($\sigma//$ parallel to the basal plane, $\sigma_\perp$ concerning the atoms out of the basal plane), the backscattering amplitudes A_T were extracted from the inverse FT of the first shell of neighbours for the two orientations at the different temperatures T.

In the case of harmonic approximation for the thermal motion, $\sigma//$ and $\sigma_\perp$ are the second moments of the gaussian distribution function of distances and the EXAFS modulation χ (k) is proportional to :

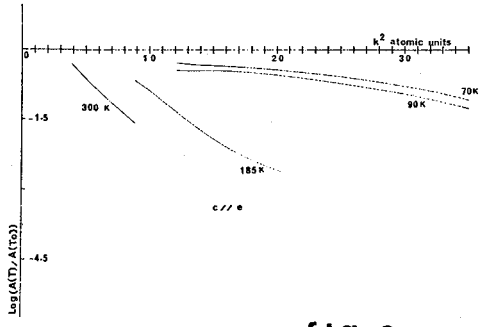
$$\sum_j \frac{N_j|f_j(k)|}{kR_j^2}\exp(-2R_j/\lambda)\exp(-2k^2\sigma_j^2)\sin[2kR_j+\delta_j(k)]$$

with R_j the mean distance between the central atom anf the $j^{\underline{th}}$ neighbours ; $\sigma_j = \sigma//$or $\sigma\perp$, θ_j the angle between the polarization vector and R_j, $\delta_j(k)$ the phase shift and λ the mean free path. For a shell of atoms having the same σ, the plot of log (A_T/A_o) versus k^2 gives a straight line, the slope of which is equal to $2(\sigma^2_T-\sigma_{T_o}^2)$. A_o is the amplitude of the filtered 1st shell at temperature T_o, A_T at temperature T. (Ratio method(7)).

The Ratio method is also used even if a non negligeable amount of anharmonicity is present. In that case, the higher order cumulants of the distribution can be extracted and

$$\mathrm{Log}(A(T)/A(T_o)) \cong 2\mathrm{Log}(R(T_o)/R(T_1)) - 2(C_2(T_1)-C_2(T_o))k^2 + 2/3C_4(T_1)k^4$$

C_2 and C_4 are cumulants of order 2 and 4 of the distribution .



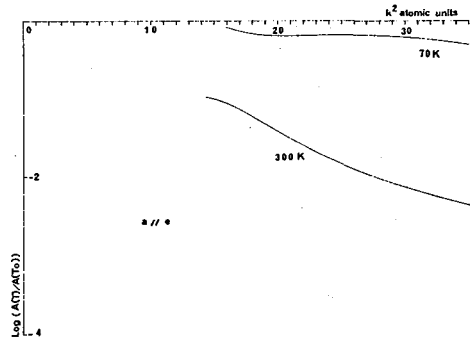


fig 3

The fig 3 shows log [A(T)/A(To)] versus k^2 at different temperatures for both orientations. In the case of a//e spectra, the contribution of the large distances was not substracted.

It can be seen in fig 3 that harmonic approximation is certainly not valid for 185k and 300k ($\sigma_\perp$), nor for 300k, σ// . However, as a first attempt of evaluating the thermal disorder, only harmonic approximation has been applied. Table I gives $\Delta\sigma$ for the two orientations and different temperatures.

T K	70	90	185	300
$\Delta\sigma_\perp$	0.06	0.07	0.12	0.14
$\Delta\sigma_{//}$	0.03			0.1

This table indicates unrealistic values for high temperatures measurements. It will be necessary to calculate higher order cumulants and to use a model of distribution of distances obtained from a knowledge of phonon distribution. In the case of $\sigma\perp$, room temperature spectra do not extend over a large energy range and such an evaluation will be difficult.

1) A. FONTAINE, E. DARTYGE, G. TOURILLON , EXAFS and NEAR Edge Structure III Ed. Hodgson Springer 1984, P 403.
2) G.S BROWN, P.EINSENBERGER, P.SCHMIDT Solid State Com. 24 201, 1977.
3) W. THULKE, P.RABE, J Phys C 16 L955 (1983)
4) A. SADOC, P.LAGARDE, G.VLAIC, J Phys.C.Sol.St.Phys 18 23 (1985)
5) J.GODARD, Laboratoire de Physique des Solides, Université Paris Sud 91405 Orsay Cedex.
6) G.BENI and P.M PLATZMAN Phys Rev B 14 1515 (1976)
7) G.BUNKER NIM, 437 (1983)