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TEMPERATURE DEPENDENCE OF THE MEAN SQUARE RELATIVE DISPLACEMENTS OF NEAREST NEIGHBOUR ATOMS DERIVED FROM EXAFS SPECTRA

by

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Temperature dependence of the mean square relative displacements of nearest neighbour atoms derived from EXAFS spectra

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Abstract

We have investigated the temperature dependence of the extended X-ray absorption finestructure (EXAFS) above the K-edges of Cu and Co in the metals and above the K-edges of Rb and Sr in the compounds RbCl, SrS, SrF_2 and $SrCl_2$. For Cu, Co, RbCl, and SrS a good agreement of the correlated mean square relative displacements of nearest neighbour atoms is observed between the values derived from EXAFS spectra and values calculated from a Debye model. Our experimental data are compared with available mean square displacements of the individual atoms calculated from more refined lattice vibrational models and with Debye-Waller factors used in X-ray diffraction experiments.

1. Introduction

The extended X-ray absorption finestructure (EXAFS) showing up above the absorption edges of atoms in molecules, liquids, and solids is caused by the interference of the outgoing photoelectron wave and parts of this wave backscattered from the neighbouring atoms (Kronig 1932, Stern 1974). There has been a renewed interest in EXAFS since methods have been developed to extract informations about local geometrical structures, i.e. bond lengths and coordination numbers from experimental spectra (Lytle et al 1975, Stern et al 1975, Rabe 1978). Whereas the periodicity of the EXAFS oscillation is determined by the bond lengths between absorbing and scattering atoms, the amplitudes of the finestructure contain informations about the number of atoms surrounding the absorbing atom. It has long been known that these amplitudes exhibit a temperature dependence which is due to thermal vibrations of absorbing and scattering atoms (Hanawalt 1931, Shmidt 1961, Shmidt 1963). At high temperatures the finestructure is damped and the energy range where EXAFS can be observed decreases. Therefore measurements are usually made at low temperatures or a precise knowledge of the atomic motions is important for reliable predictions of coordination numbers from EXAFS.

We have measured the variation of this finestructure with temperature above the K-edges of Cu, Co, Rb in RbCl as well as Sr in SrS, SrF_2, and $SrCl_2$. In the next section we shall briefly describe our experiment. In section 3 we present our results and compare them with i) calculations for Debye-Waller factors performed within the Debye model, ii) other published data of the atomic motions calculated from more refined lattice dynamical

models, and iii) values used in X-ray diffraction experiments.

2. Experiment

The absorption spectra of Cu and Co have been measured at the Deutsches Elektronen-Synchrotron DESY. The synchrotron radiation was monochromatized with a channelcut Ge (111)-crystal. The monochromatic radiation was monitored by airfilled ionization chambers. The signals were digitized and stored in a computer. Details about this experimental setup will be published elsewhere (Rabe et al 1978). For the investigation of the other samples we used a 12 kW X-ray generator with rotating Ag- and Au-anodes as light source. The bremsstrahlung was monochromatized by a LiF (200) crystal and detected with a NaI(Tl) scintillation counter.

The samples were mounted in a liquid nitrogen cryostat. The temperature of the samples was varied between 80 K and 420 K. The Cu sample was prepared as 4 μm thick unsupported foil by vacuum evaporation. The other samples have been powdered from polycrystalline material. They were enclosed between adhesive tape and a thin aluminium foil to ensure good thermal contact with the cryostat.

3. Results and discussion

For polycrystalline materials the oscillatory part of the absorption coefficient above K-edges is described by

$$1) \quad \chi(k) = -\frac{1}{k}\sum_i A_i(k)\sin(2kR_i + \Phi_i)$$

with

$$2) \quad A_i(k) = \frac{N_i}{R_i^2}\left|f_i(\pi,k)\right|\exp(-2R_i/\lambda)\exp(-2\sigma_i^2 k^2)$$

Here k denotes the wave number of the photoelectrons, Φ_i the scattering phase, and R_i the bond length between the absorbing atom and the scattering atom in the i-th shell. The amplitude function $A_i(k)$ contains as correlated variables the coordination numbers N_i, the backscattering amplitudes $|f_i(\pi, k)|$ of the photoelectronwave, the mean free path λ for inelastic scattering of the photoelectrons and the temperature dependent mean square relative displacements σ_i^2.

The procedure to evaluate changes of σ_i^2 with temperature for a single scattering shell will be demonstrated on the EXAFS spectra of Cu. The finestructure measured at 8o K and 42o K are shown in Fig. 1. The monotonous contribution to the absorption coefficient due to excitations of K-shell and weaker bound electrons has been removed by a procedure described elsewhere (Martens et al 1978). For the conversion of the energy scale to the k-scale the energy zero was taken at one half the step height of the absorption edge. The damping of $\chi(k)$ at large k values and the broadening of structures at high temperatures is apparent from inspection of Fig. 1. According to eq. 1 these spectra represent a superposition of contributions from different scattering shells so that detailed informations about the temperature dependence of EXAFS, i.e. the values of the mean square relative displacements σ_i^2 of individual atom pairs cannot be extracted from the amplitudes of $\chi(k)$ directly.

In order to separate the single shell contributions we have performed a Fourier transform to real space. All spectra except Cu and Co have been weighted with a Caussian window function. The effect of this window is a considerable reduction

of truncation effects in the Fourier transform, although this weighting results in a slight broadening of structures in real space due to the effectively smaller k range (Gurman and Pendry 1976, Martens et al 1978). As a result we show the magnitude of the Fourier transform $|F(r)|$ of the two spectra of Cu taken at 80 K and 42o K in Fig. 2. In this figure five peaks can be identified which are attributed to the first five nearest neighbour shells surrounding the absorbing atom. Compared to the true distances the positions of these peaks are shifted due to the k dependent parts of the scattering phase $\Phi(k)$. Each maximum has been labelled with the number of scattering atoms in the attached shell. The decreasing contribution from more distant shells even in $|F(r)|$ calculated from the low temperature data is caused by the damping of the photoelectron wave by inelastic scattering processes. The additional damping in $|F(r)|$ derived from the high temperature spectrum originates from the atomic vibrations and results in a significant loss of informations for more distant shells.

The widths and amplitudes in real space are determined by the effective range in k space where EXAFS shows up with significant amplitudes, the transformation window, and the spectral resolution. To avoid influences of these parameters on the determination of differences in the mean square relative displacements $\Delta\sigma_i^2$ we interpret our data in k space. For this purpose we have transformed back to k space over a limited range in real space, as indicated by a bar for the first scattering shell of Cu in Fig. 2. According to the window function used for the transformation to real space, i.e. due to the reduction of truncation effects, the informations about the amplitude functions

$A_i(k)$ and the scattering phases $\Phi_i(k)$ are concentrated in this range of $F(r)$. The result of this backtransform is the contribution from one single shell to $X(k)$. Applying this procedure to spectra taken at different temperatures T_1 and T_2, changes of the mean square relative displacements of single atom pairs can simply be calculated by

$$(3) \quad \Delta\sigma^2_{EXAFS} = \sigma^2_{T_1} - \sigma^2_{T_2} = (2k^2)^{-1} \ln\left[A_{T_2}(k)/A_{T_1}(k)\right]$$

The results of $\Delta\sigma^2_{EXAFS}$ should be a constant over the whole k range. Due to the small thermal expansion of the lattice the influence of changes in R with temperature on $\Delta\sigma^2_{EXAFS}$ calculated from eq. 3 can be neglected. The deviations from a constant value which are mainly due to residual truncation effects in the Fourier transform have to be regarded as the uncertainties of our results. All values of $\Delta\sigma^2_{EXAFS}$ determined in this way are summarized in Table 1 column VII .

For a monoatomic lattice the mean square relative displacements of atom pairs with relative distances R_j in a crystal can be described by (Warren 1969, Beni and Platzman 1976).

$$4) \quad \sigma_i^2 = \frac{2\hbar}{NM} \sum_{\vec{q}\lambda} \frac{\lambda}{\omega_{\vec{q}\lambda}} \left[n(\omega_{\vec{q}\lambda}) + \frac{1}{2}\right]\left[1-\cos(\vec{q}\vec{R}_i)\right]$$

with $n_{\vec{q}\lambda}$ the phonon occupation number and N the number of atoms with mass M. The phonons are represented by their polarization vector $e_{\vec{q}\lambda}$, the momentum $\vec{q}$, the polarization λ, and the frequency $\omega_{\vec{q}\lambda}$. For completely uncoupled motion σ_i^2 approaches to twice the mean square displacement σ_∞^2 of the individual atoms. The correlation between the atomic motions which is most dominant for the nearest neighbour atoms is taken into account by the last term ($\cos \vec{q}\cdot\vec{R}_j$). This term describes the in-phase motions of the atoms which do not affect the amplitudes of EXAFS.

Using the Debye approximation, σ_i^2 as a function of temperature T can be represented by (x)

$$(5) \quad \sigma_i^2 = 2\,\sigma_\infty^2\,(1 - \gamma)$$

$$(6) \quad \sigma_\infty^2 = \frac{3\hbar}{M\omega_D}\left[\frac{1}{4} + \left(\frac{T}{\theta}\right)^2 \Phi_1\right]$$

$$(7) \quad \gamma\sigma_\infty^2 = \frac{3\hbar}{M\omega_D}\left[\frac{1 - \cos(q_D R_i)}{2(q_D R_i)^2} + \left(\frac{T}{\theta}\right)^2 \sum_{n=o} \frac{(-1)^n}{(2n+1)!}\left(q_D R_1 \frac{T}{\theta}\right)^{2n} \Phi_{2n+1}\right]$$

with

$$(8) \quad \Phi_n = \int_o^{\theta/T} \frac{x^n}{e^x - 1}\,dx$$

Here ω_D means the Debye cut-off frequency, θ the Debye temperature, q_D the Debye wavenumber and $\gamma\sigma_\infty^2$ describes the in-phase motion of the atoms. Although eq. 5 is strictly valid only for monoatomic cubic crystals we have calculated the temperature dependence of σ_i^2 from eq. 5 for all investigated materials. For the binary compounds RbCl, SrS, SrF_2, and $SrCl_2$ we have approximated the atomic mass M by the average mass of the individual ions. The Debye temperatures θ , the distances of the atom pairs R_i, and the $q_D R_i$ values are compiled in

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(x) Compared to eq. 19 of Beni and Platzmann (1976) an additional factor of 2 had to be included in eq. 5 for completeness.

Table 2. A comparison of the measured differences of the mean square relative displacements $\Delta\sigma^2_{EXAFS}$ with the calculated values $\Delta\sigma^2$ (Table 1, column VI and VII) shows a good agreement for the first and second scattering shell of Cu, Co and the first shell of $RbCl_2$. Compared to the magnitude of $\Delta\sigma^2_{EXAFS}$ a large experimental uncertainty exists in the case of $SrCl_2$. For Cu, Co, and RbCl the temperature dependence of σ^2_i up to 600 K are shown in Fig. 3. Our experimental $\Delta\sigma^2_{EXAFS}$ which are included in this figure have been fitted to the theoretical value of σ^2_i at 80 K. Again the result shows that the data derived from the EXAFS spectra follow the calculated curves within the experimental uncertainties.

For SrS the calculated value is smaller than the experimental $\Delta\sigma^2_{EXAFS}$. This fact is certainly due to a too high Debye temperature used in our calculation. The Debye temperature of chalcogenide crystals with sodiumchloride structure has been calculated by Thakur (1977) using a logarithmic interaction potential energy function. Compared to values of Θ estimated for alkaline earth chalcogenides by Huggins and Sakamoto (1957) the model of Thakur (1977) seems to overestimate the Debye temperature. Using the value of Huggins and Sakamoto (1957) for the calculation of σ^2_i from eq. 5 our experimental result agrees with the calculated $\Delta\sigma^2_i$. The mean square relative displacement of the nearest neighbour atoms in SrS has been included in Fig. 3.

For SrF_2 we find an experimental $\Delta\sigma^2_{EXAFS}$ which is not reproduced by eq. 5 using the Debye temperature of Brade and Yates (1969). Whether this difference is due to incorrect Debye temperature or due to an incorrect estimation of the correlation in this crystal is not evident. In this case a more detailed analysis

of the lattice dynamical properties seems to be necessary which is beyond the scope of this paper.

For RbCl, Cu, and Co we have compared our data with available mean square displacements calculated from more refined lattice dynamical models. Using shell models the temperature dependence of the mean square displacements of the ions have been calculated by Govindarajan (1973) and Gupta (1975) for RbCl. From these values we have calculated the mean square relative displacements of the nearest neighbour Rb and Cl ions by subtracting the in-phase motion of the ions using the displacement correlation function (eq.7) . In both cases the results which are included in Fig. 3 are close to the values obtained within the Debye approximation and close to our experimental data. This means that the temperature dependence of the uncorrelated mean square displacement calculated within the Debye approximation is in agreement with the results of Govindarajan (1973) and Gupta (1975).

Applying the same correction to the theoretical values of Cu as discussed above for RbCl we find a good agreement between our data and the results of Sinha (1966) whereas the values of Kharoo et al (1977) are too large for both scattering shells (Table 1). Using eq. 4 the mean square relative displacements for Cu have been calculated by Sevillano et al (1978). The results which are included in Table 1 are in excellent agreement with the experimental values.

It should be noted at this point that the ratio γ of the displacement correlation function and the mean square displacement shows a significant temperature dependence. This ratio calculated from eq. 7 is shown in Fig. 4 as a function of q_DR for various $^T/_\Theta$ values. The q_DR values of the first shells in a fcc lattice are indicated by arrows. At high temperatures γ approaches to 0.38 for the nearest neighbours. With decreasing temperature and increasing distance of the atom pairs the correlation decreases. The oscillations in γ as a function of q_DR are caused by the zero-point vibrations in the lattice. This effect should be observable at low temperatures ($^T/_\Theta < 0.1$) by a comparison of σ_i^2 for nearest and next nearest neighbours.

In Table 1 column IV we have compiled the available data of the mean square displacements of the individual atoms used in X-ray diffraction experiments of Cu, Co, and $SrCl_2$. In the same way as for EXAFS the decrease of X-ray diffraction maxima with temperature can be expressed by an exponential factor $\exp(-2B((\sin\vartheta)/\lambda)^2)$ where λ is the wavelength and ϑ the Bragg angle. The relation between the exponent and the component of uncorrelated mean square displacement along the line of two atoms σ_∞^2 is given by

$$(9) \qquad B = 8\pi^2 \sigma_\infty^2$$

The correlated motion of close lying atoms manifests itself in X-ray diffraction in a thermal diffuse scattering intensity (Azaroff et al 1974, Warren 1969, Walker and Keating 1961) which has to be taken into consideration in the evaluation of high precision structural data from single crystal and powder diffraction pattern. The mean square relative displacements σ_i^2 derived from EXAFS data may therefore be used as input parameters for the analysis of X-ray diffraction data. We have corrected the σ_∞^2 from X-ray diffraction by the displacement correlation function (eq. 7). The resulting values of $\Delta\sigma_i^2$

shown in Table 1 are close to our experimental results. For the second scattering shell of Cu our EXAFS value is slightly larger than the X-ray diffraction value. For Co the diffraction value for the first scattering shell is close to the upper limit of the EXAFS value whereas $\Delta\sigma^2$ for the second shell is larger than our result. This may indicate that the amplitudes of the thermal vibrations of the Co atoms have been overestimated in the diffraction data.

For the first scattering shell of Cu we have determined the absolute value of σ_1^2 at 80 K by the following procedure: Using the magnitude of the complex backscattering amplitude $f(\pi, k)$ calculated by Teo and Lee (1978) the amplitude function $A_1(k)$ has been calculated. It is well known that the theory overestimates the magnitude of $f(\pi,k)$ (Lee and Beni 1977). Therefore an overall scaling factor for $|f(\pi,k)|$ and the mean square relative displacement σ_1^2 have been varied in a way to give a best fit of the calculated with our experimental amplitude function $A_1(k)$. The result yields a scaling factor of 0.59 and $\sigma_1^2 = (0.36 \pm 0.03)\ 10^{-22}m^2$ compared to $0.3548 \cdot 10^{-22}m^2$ calculated from the Debye model. The good agreement of these values justifies the fit of our experimental $\Delta\sigma^2_{EXAFS}$ to the calculated σ_i^2 curves at 80 K in Fig. 3.

By fitting the full EXAFS spectrum Gurman and Pendry (1976) obtained values for σ_i^2 for the first five shells in Cu at 80 K. For the first two shells treated in this work they found $\sigma_1^2 = (0.36 \pm 0.014) \cdot 10^{-22}m^2$ and $\sigma_2^2 = (0.38 \pm 0.07) \cdot 10^{-22}m^2$. A value of $\Delta\sigma^2 = (0.47 \pm 0.04) \cdot 10^{-22}m^2$ between 77 K and 300 K has been reported by Stern at al (1975) for the first shell. All these values are in excellent agreement with our results.

4. Conclusions

The good agreement between mean square relative displacements of atom pairs in crystals derived from EXAFS data und values calculated within the Debye approximation shows that the correlated motion between nearest neighbour atoms is correctly taken into account by this simple model. Without knowledge of the dependence on the electron wavenumber k of all parameters which influence the amplitudes of EXAFS it is difficult if not impossible to extract coordination numbers from experimental spectra. The fact that the Debye model yields reliable predictions of the temperature dependence of EXAFS, in many cases opens simple ways to account for thermal broadening and damping. This fact facilitates the evaluation of coordination numbers around specific atoms. Certainly the Debye approximation yields an adequate description of the vibrational properties only for simple crystal structures. For more complex structures or crystals with strong covalent bonding character the description of the correlation in various shells may demand a more realistic model. Nevertheless values of the mean square relative displacements evaluated from EXAFS spectra could be used in various fields as force model calculations or structural analysis from X-ray diffraction.

An additional damping of the EXAFS oscillations may be due to a static structural disorder in solids. The superposition of contributions from close lying scattering shells to EXAFS leads to a k dependent damping of the EXAFS amplitudes (Martens et al 1977) which may be difficult to distinguish from the thermal disorder at a definite temperature. In these cases a distinction between the dynamic thermal disorder and the static structural disorder can be made from the temperature dependence of EXAFS.

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References

American Institute of Physics Handbook (1963) Table 4 e-12 (Mc Graw-Hill, New York)

Azaroff L V, Kaplow R, Kato N, Weiss R J, Wilson, A J C and Young R A (1974) X-Ray Diffraction (Mc Graw-Hill, New York)

Beni G and Platzman P M (1976) Phys. Rev. B14, 1514-1518

Brade R M and Yates B (1969) phys.stat.sol. 36, 551-556

Flinn P A, Mc Manus G M and Rayne J A (1961) Phys.Rev. 123, 809-812

Govindarajan J (1973) Acta Cryst. A29, 576-577

Gupta R K (1975) Phys.Rev. B12, 4452-4459

Gurman S J and Pendry J B (1976) Solid State Commun. 20, 287-290

Hanawalt J D (1931) Z.Phys. 70, 293-305

Huggins M L and Sakamoto Y (1957) J.Phys.Soc. Japan 12, 241-251

International Tables for X-Ray Crystallography (1968) Vol.III, Table 3.3.5.1B. and C. (Kynoch Press, Birmingham) and references therein

Järvinen M and Inkinen O (1967) phys.stat.sol. 21, 127-135

Kharoo H 1 Gupta O P and Hemkar M P (1977) Z. Naturforsch. 32a, 570-576

Kronig R de L (1932) Z.Phys. 75, 468 - 475

Lauer H V, Solberg K A, Kühner D H and Bron W E (1971) Phys.Letters 35A, 219-220

Lee P A and Beni G (1977) Phys. Rev. B15, 2862-2883

Linkoahoa M, Rantavuori E, Korhonen U, Kurki-Suonio K and Ruuskanen A (1972) Acta Cryst. A28, 260-264

Lytle F W, Sayers D E and Stern E A (1975) Phys.Rev. B11, 4825-4835

Martens G, Rabe P, Schwentner N, and Werner A (1977) Phys. Rev. Letters 39, 1411-1414

Martens G, Rabe P, Schwentner N and Werner A (1978) Phys. Rev. B17, 1481-1488

Pathak P D and Trivedi J M (1973) Acta Cryst. A29. 45-49

Rabe P (1978) Jap.J.Appl.Phys.

Rabe P, Tolkiehn G and Werner A (1978) to be published

Sevillano E, Rehr J and Meuth H (1978) to be published

Shmidt V V (1961) IZV.Akad.Nauk.SSSR 25, 977-982

Shmidt V V (1963) IZV.Akad.Nauk.SSSR 27, 384-389

Sinha S K (1966) Phys.Rev. 143, 422-433

Stern E A (1974) Phys.Rev. B10, 3027-3037

Stern E A, Sayers D E and Lytle F W (1975) Phys. Rev. B11, 4836-4846

Teo B-K and Lee P A (1978) to be published

Thakur K P (1977) Austr.J.Phys. 30, 325-334

Walker C B and Keating D T (1961) Acta Cryst. 14, 1170-1176

Warren B E (1969) X-Ray Diffraction (Addison-Wesley, Reading)

I	II	III	IV		V			VI	VII
			σ_∞^2 [$10^{-22}m^2$]		σ_i^2 [$10^{-22}m^2$]			$\Delta\sigma^2$ [$10^{-22}m^2$]	$\Delta\sigma^2_{EXAFS}$ [$10^{-22}m^2$]
	shell	ref.	80K	300K	80K	300K	420K		
Cu	1	1	0.25	0.67	0.36	0.84		0.48	0.48 ± 0.04
		3	0.19	0.73	0.28	0.92		0.64	
		4	0.246	0.685	0.351	0.857		0.605	
		DM			0.3548	0.8676		0.5098	
		5			0.328	0.770		0.442	
		DM			0.3578		1.0754	0.7176	
		5			0.328		1.065	0.737	0.74 ± 0.08
	2	1			0.43	1.04		0.61	0.71 ± 0.09
		3			0.33	1.13		0.80	
		4			0.421	1.059		0.638	
		DM			0.4288	1.0793		0.6505	
		5						0.68	
Co	1	1	0.19	0.49	0.29	0.63		0.34	0.25 ± 0.10
		DM			0.2532	0.5047		0.2515	
	2	DM			0.2994	0.6162		0.3168	0.30 ± 0.10
		1			0.34	0.78		0.44	
RbCl	1	6	0.778	2.951	1.030	3.651		2.621	2.2 ± 0.4
		7	0.75	2.52	0.99	3.12		2.13	
		DM			1.1197	3.5924		2.4727	
SrS	1	DM (= 404K)			0.2798	0.5939		0.3141	0.53 ± 0.08
		DM (= 337K)			0.3517	0.8348		0.4831	
SrF_2	1	DM			0.4520	1.0812		0.6292	0.46 ± 0.08
$SrCl_2$	1	DM			0.3439	0.7613		0.4174	0.70 ± 0.37
		2	0.37	1.16	0.57	1.47		0.90	

Table 1

Table 1: Compilation of the uncorrelated mean square displacements σ_∞^2 used in X-ray diffraction experiments ((1) Int. Tables (1968), (2) Linkoahoa (1972)) and calculated from various lattice vibrational models ((3) Kharoo et al (1977), (4) Sinha (1966), (5) Sevillano et al (1978), (6) Govindarajan (1973), (7) Gupta (1975)), of mean square relative displacements σ_i^2 calculated from σ_∞^2 by subtracting the in-phase motion of the atoms and of values calculated from the Debye model (DM). In column VI and VII the variation of σ_i^2 between 80 K and 300 K / 420 K are compared with our experimental $\Delta\sigma^2_{EXAFS}$.

Table 2: Crystal structures, bond lengths R_i of nearest neighbours, q_DR_i values and Debye temperatures Θ used for the calculation of the mean square relative displacements from eq.5. The Θ values have been taken from (1) Flinn et al (1961), (2) AIP Handbook (1963), (3) Pathak and Trivedi (1973), (4) Järvinen and Inkinen (1967), (5) Thakur (1977), (6) Huggins and Sakamoto (1957), (7) Brade and Yates (1969), and (8) Lauer et al (1971).

	Structure	shell i	R_i [10^{-10} m]	$q_D R_i$	Θ [K]		
					80 K	300 K	420 K
Cu	fcc	1	2.556	4.375	318 (1)	320 (1)	320
		2	3.615	6.187			
Co	hcp	1	2.507	4.375	445	445 (2)	
		2	3.546	6.187			
RbCl	NaCl	1	3.291	4.375	157	157 (3,4)	
SrS	NaCl	1	3.010	4.375	404	404 (5)	
					337	337 (6)	
SrF_2	CaF_2	1	2.510	4.375	366 (7)	355 (7)	
$SrCl_2$	CaF_2	1	3.022	4.375	378	378 (8)	

Table 2

Figure Captions

Fig.1: EXAFS spectra above the K edge of Cu at 80 K and 420 K

Fig.2: Magnitude of the Fouriertransform of the EXAFS spectra of Cu at 80 K and 420 K

Fig.3: Temperature dependence of the mean square relative displacements σ_i^2 for the first and second scattering shell of Cu and Co and the first shell of RbCl and SrS calculated from eq.5. The crosses and circles are the results of Govindarajan (1973) and Gupta (1975) for RbCl after subtraction of the displacement correlation function (eq.7). The EXAFS results have been fitted to the values calculated from the Debye model at 80 K.

Fig.4: Ratio of the displacement correlation function and the mean square displacement for various values of T/Θ as function of q·R. The positions of the first 13 shells in a hcp lattice have been indicated by arrows.

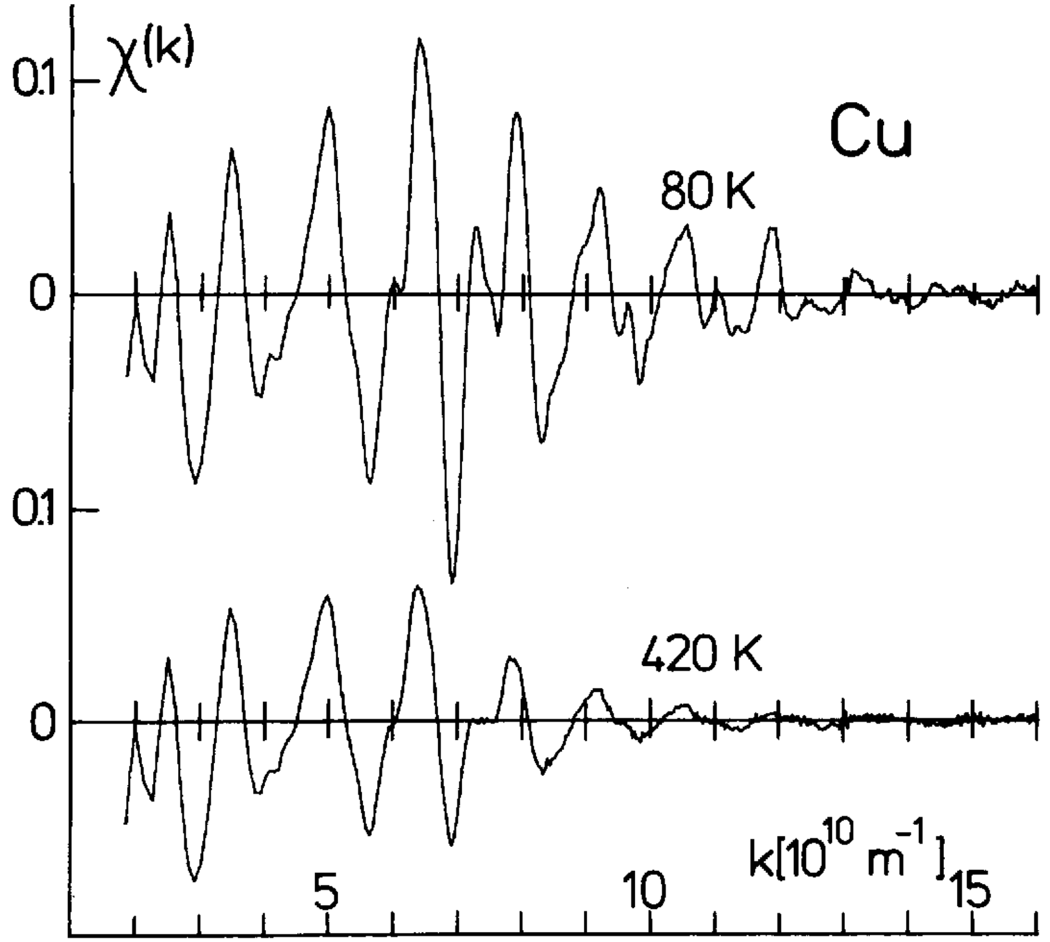
0.1
χ(k)
Cu
80 K
0
0.1
420 K
0
5
10
k[10^10 m^-1]
15

Fig.1

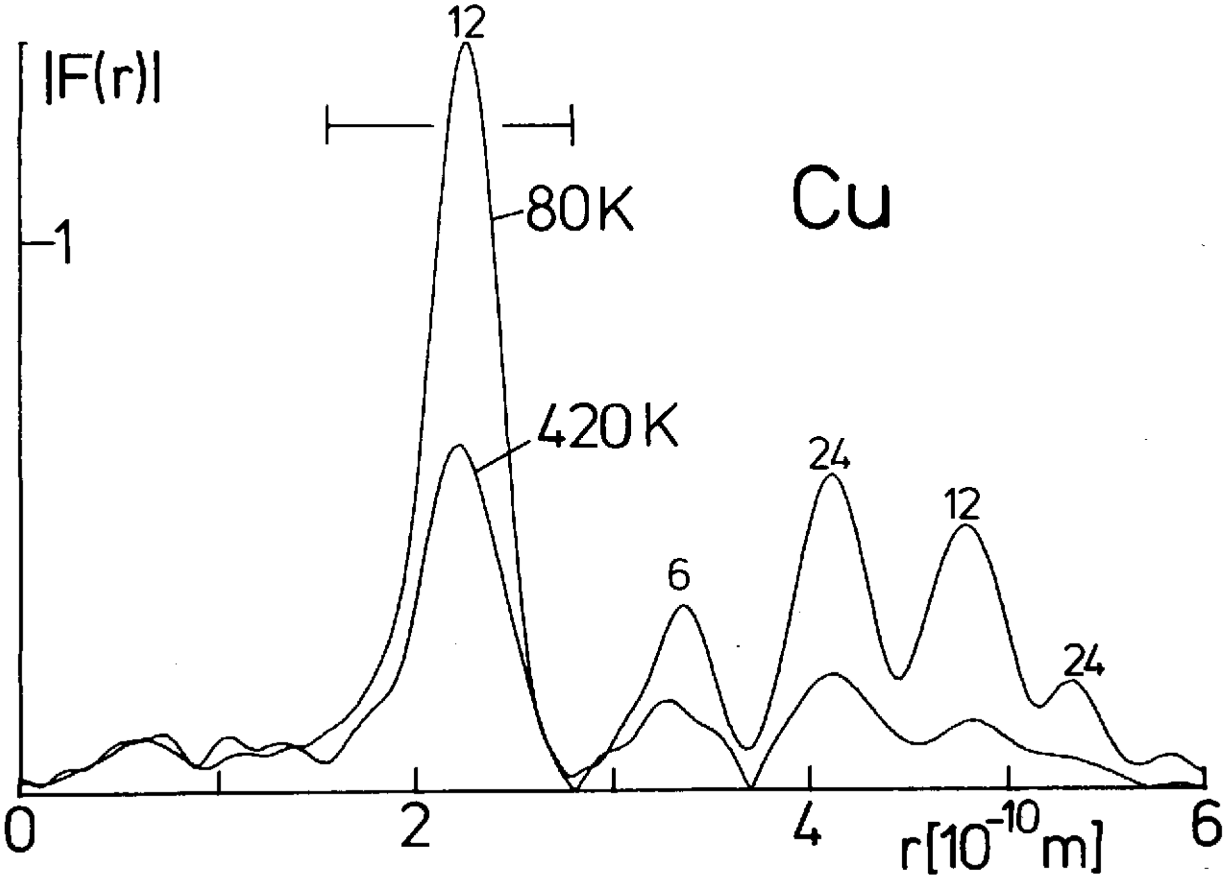
12
|F(r)|
80K
Cu
1
420K
24
6
12
24
0
2
4
r[10^-10 m]
6

Fig. 2

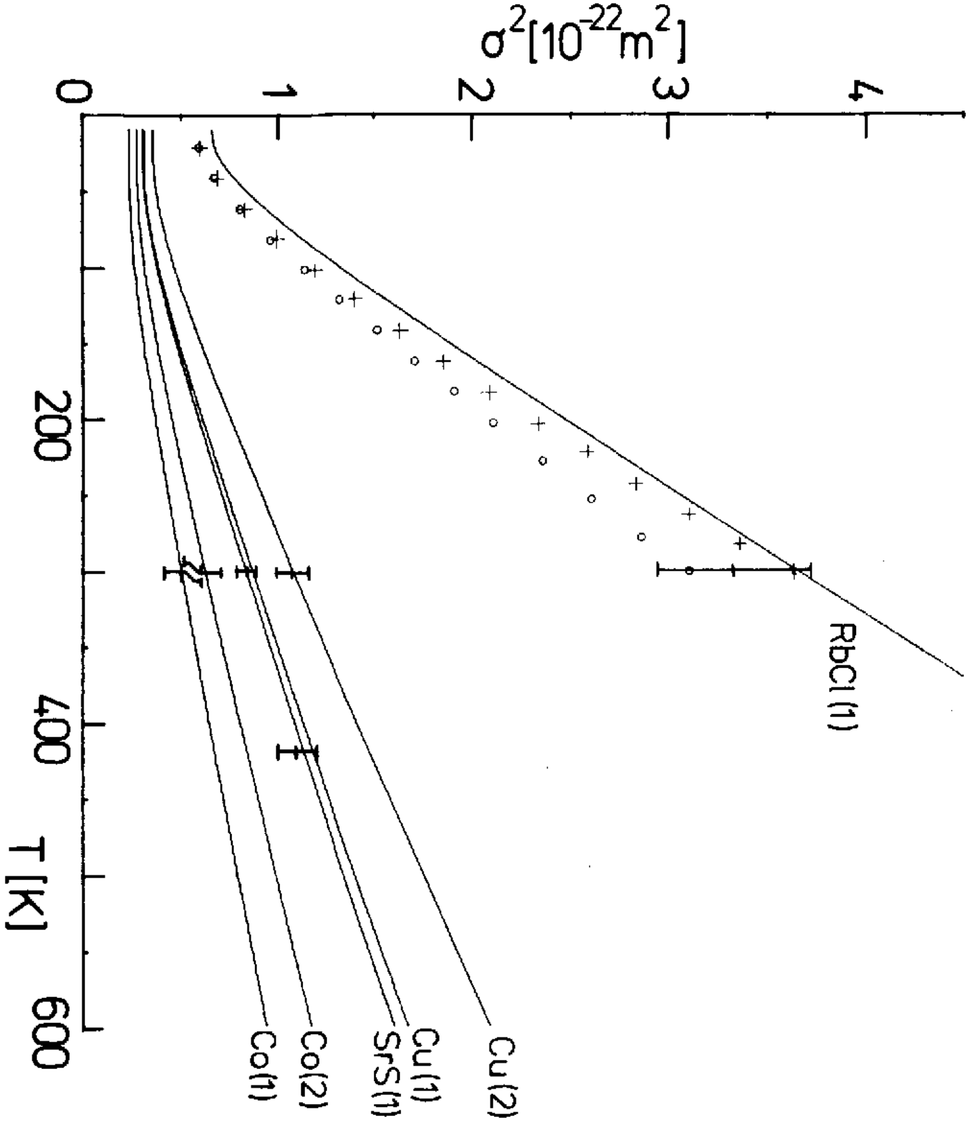
$\sigma^2 [10^{-22} m^2]$
0
1
2
3
4
200
400
600
T [K]
RbCl (1)
Cu (2)
Cu (1)
SrS (1)
Co (2)
Co (1)

Fig. 3

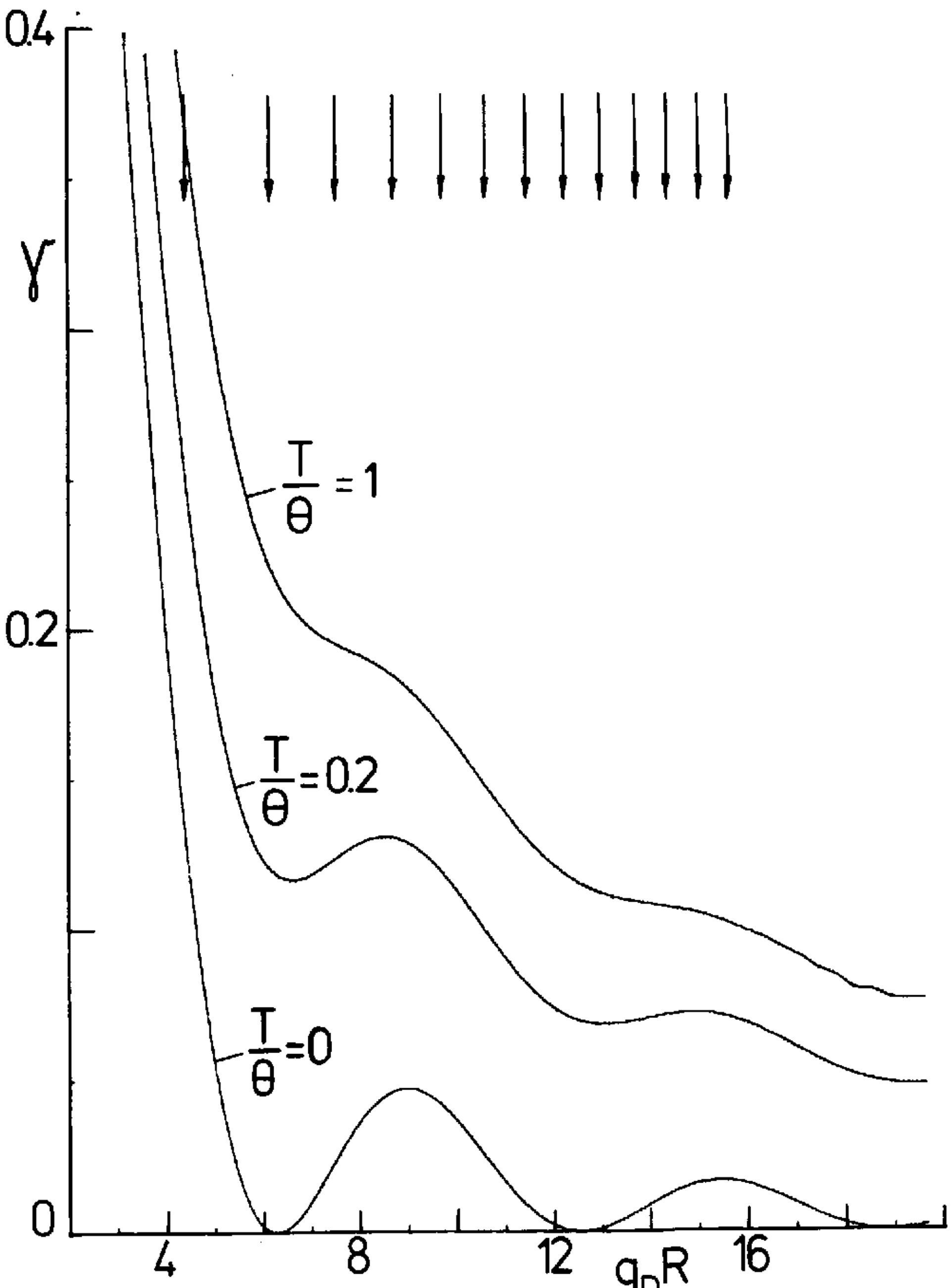
0.4
0.2
0
γ
$\frac{T}{\theta} = 1$
$\frac{T}{\theta} = 0.2$
$\frac{T}{\theta} = 0$
4
8
12
16
$q_D R$

Fig. 4