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## EXAFS in Photoelectron Yield Spectra at K Edges of Cu, Ni and Ge

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### Abstract

The total photoelectron yield as a function of the photon energy of poly- and singlecrystalline Ni and Ge and of thin films of Cu on Ni has been measured at the K absorption edges and compared with the absorption coefficient. The data are discussed considering the relative contribution of the electron cascades caused by Auger- and photoelectrons to the yield and the information depth of the yield EXAFS method.

Die totale Photoelektronenausbeute von poly- und einkristallinem Ni and Ge und von dünnen Schichten von Cu auf Ni wurde im Bereich der Absorptions-K-Kanten gemessen und mit dem Absorptionskoeffizienten verglichen. Die Daten werden bezüglich der relativen Beiträge der von Auger- und Photoelektronen ausgelösten Elektronenkaskaden sowie der Informationstiefe der Ausbeute EXAFS Methode diskutiert.

The investigation of the extended x-ray absorption fine structure (EXAFS) has become a powerful tool for the analysis of the local geometrical structure of atoms in polyatomic systems. In the recent years, much experimental work has been done to measure EXAFS by various techniques [1, 2]. Here we present measurements of the K edge EXAFS of Ge, Ni and Cu-Ni systems which are related to previous work on Cu yield EXAFS [3]. In this paper we discuss (i) the relative contribution of electron cascades caused by primary Auger and photoelectrons to the total yield, (ii) the influence of direction dependent emission probability of photoelectrons on yield EXAFS and (iii) the information depth of the yield method.

The yield spectra have been measured at the synchrotron radiation facility of the Deutsches Elektronen-Synchrotron DESY at Hamburg. The experimental arrangement consists of an x-ray monochromator with channel-cut Si (220) and Ge (111) crystals for the spectral range from 5 keV to 28 keV. The primary intensity is monitored by an ionization chamber. The degree of polarization amounts to well over 90%. In order to exclude influences on the EXAFS due to different orientations of the polarization vector relative to the crystallographic axes [4], we have chosen samples with cubic symmetry. An ultra-high vacuum sample chamber with a base pressure of less than $10^{-10}$ mbar allows the preparation of the sample by heat treatment, Argon ion sputtering, and vacuum evaporation. The surface quality can be controlled by LEED. The x-rays enter the chamber through a Be window. The electrons are monitored by an electron multiplier.

In Fig. 1a, b the absorption coefficients of polycrystalline Ge and Ni are compared with the yield spectra of single crystal Ge (111), single crystal Ni (111) and polycrystalline Ni. It is worth noting that the energy positions of the half step height of the K edge of both the Ge and Ni yield spectra coincide with the respective absorption edge within the resolution of the monochromator of about 1 eV. This holds also for the K edge of the Cu spectra reported elsewhere [3]. The

near edge structures of Ge are compared in Fig. 1a. These results lead to the conclusion that the main contribution to the total yield consists of the cascades of secondary electrons of primary Auger electrons and reabsorbed x-ray fluorescence photons. A considerable contribution of direct photoelectrons and their secondaries at the K edge energy would have shifted the edge towards higher excitation energies compared with the absorption case due to the work functions of the samples which are approximately 5 eV for Cu, Ni and Ge [5]. A significant contribution of the primary photoelectrons and their secondaries to the total yield is expected several tens of eV beyond the edge. There the energy of the primaries is sufficient to produce an electron cascade that reaches the surface from deeper regions of the sample. This results in the observed monotonously increasing contribution to the total yield with increasing photon energy in comparison to the absorption coefficient (Fig. 1a).

As an example the fine structure $\chi(k)$ beyond the Ni K edge is shown in Fig. 2 versus photoelectron wave number k. All spectra have been handled in the same way by techniques described in detail in Ref. 1. Compared to the absorption spectra, an overall reduction of the yield amplitudes is observed for Ni as well as for Ge and Cu [3]. This fact, which has not been understood until now, has no influence on the determination of bond lengths by the EXAFS method as can be seen from the positions of the zeros of the fine structures (Fig. 2). Due to the fact that the outgoing photoelectron wave and parts of it scattered at the neighboring atoms interfere outside of the sample, an additional contribution to the EXAFS is expected [6]. It depends on the wavevector k and the direction of detection and will in general not be proportional to the normal EXAFS. As can be seen from Fig. 1, 2, the fine structures observed in the absorption and yield spectra are virtually identical for each material. This again is explained by the fact that only a small contribution to the total yield is based on photoelectrons. In addition, the scattering of the photoelectrons inside the sample and the collection of the electrons by an accelerating potential outside the sample cause an averaging of their angular distributions over almost $4\pi$ of the solid angle which is essential for reproducing EXAFS in the photoelectron yield [6].



A further argument for reproducing EXAFS in total yield spectra results from the information depth of the sample. It is well known that the attenuation length of electrons (0 eV to 2000 eV) in the bulk ranges from 5 Å to 20 Å for the individual electron [7]. Based on measurements of the dependence of the yield on the angle of incidence of the x-rays, for the whole electron cascade attenuation lengths of 1000 Å to 2000 Å have been reported [3]. This results in an information depth for structural analysis by yield EXAFS of the same order. We have checked these large information depths by the overlayer technique. Measurements of the yield for overlayer thicknesses between 30 Å and 1000 Å have been performed on Cu coverages on Ni and Ta substrate. As an example we show a yield spectrum of 100 Å Cu on a Ni substrate in Fig. 3a. The insert Fig. 3b displays the Cu EXAFS which, as well as the fine structure of the Ni substrate, is identical to bulk K edge EXAFS [1,3]. From this spectrum we have performed a Fourier transform, the magnitude $|F(r)|$ of which yields a radial structure function (Fig. 3c). A comparison with bulk Cu shows that the nearest neighbor distance is conserved in the thin film. A slight broadening of the structures in $|F(r)|$ is due to the limited range in k space where the EXAFS exceeds the noise level.

In Fig. 4 we have summarized the variation of the relative step height of the Cu K edge which is defined as the ratio of the increase of the yield due to the Cu K edge to the yield in front of the edge. We have included results for different attenuation lengths L of the electron cascades calculated within a model which is based on the assumption that the electrons are emitted from the absorbing atom isotropically and that the attenuation of the electron cascade can be described by an exponential damping with mean free path L. This model was used for the description of the dependence of the yield on the photon glancing angle [3]. The result shows that this model cannot describe the thickness dependence of the yield over the whole range of measured thicknesses. The total yield for overlayer thicknesses up to 200 Å is well described by L = 500 Å. The yields for overlayers of more than 200 Å require attenuation lengths of 1000 Å to 2000 Å in order to be described reasonably. This also holds for the step height of the K edge of the Ni substrate. The conclusion is that in agreement with former measurements the information

depth of the yield method amounts to 1000 Å. This large value is caused by the large kinetic energy of the hot primary Auger electrons from which the yield mainly originates as stated above.

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Figure captions

Fig. 1a Absorption coefficient of polycrystalline Ge and total photoelectron yield of single crystal Ge (111) as function of photon energy E. The estimated contribution of the total yield is indicated by the hatched area. In the insert the near edge structures of both spectra are compared.

Fig. 1b Absorption coefficient of polycrystalline Ni and the total yield spectra of single crystal Ni (111) and polycrystalline Ni as function of photon energy.

Fig. 2 Normalized EXAFS $\chi(k)$ of the
a) absorption coefficient of polycrystalline Ni
b) total yield of single crystal Ni and
c) total yield of polycrystalline Ni versus photoelectron wave number k.

Fig. 3 a) Total photoelectron yield spectrum of an 100 Å Cu layer on polycrystalline Ni substrate.
b) Normalized EXAFS $\chi(k)$ of the Cu K edge.
c) Magnitude $|F(r)|$ of the Fourier transform of the Cu K edge EXAFS.

Fig. 4 Dependence of the relative Cu K edge step height as function of the thickness d of the Cu overlayer on Ni substrate. Model calculations for different attenuation lengths L of the electron cascades are included as solid lines.

Fig. 1a

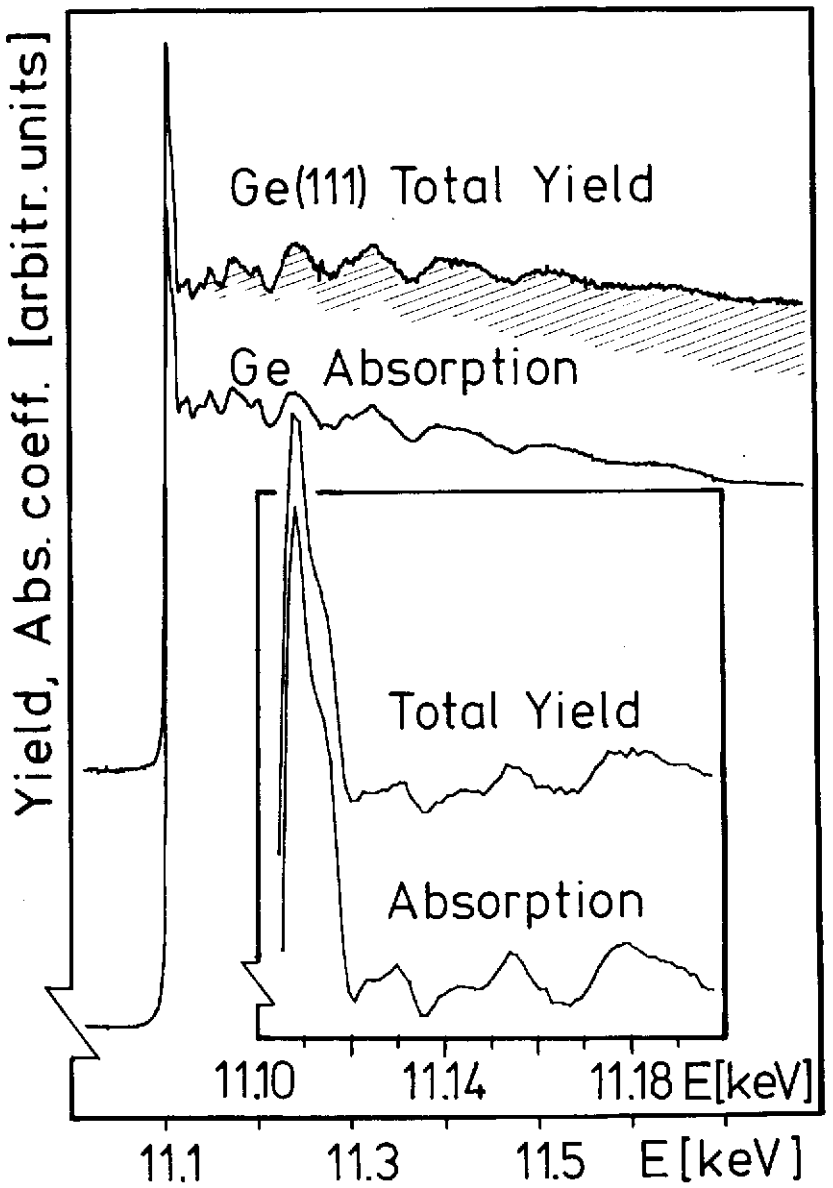


Fig. 1b

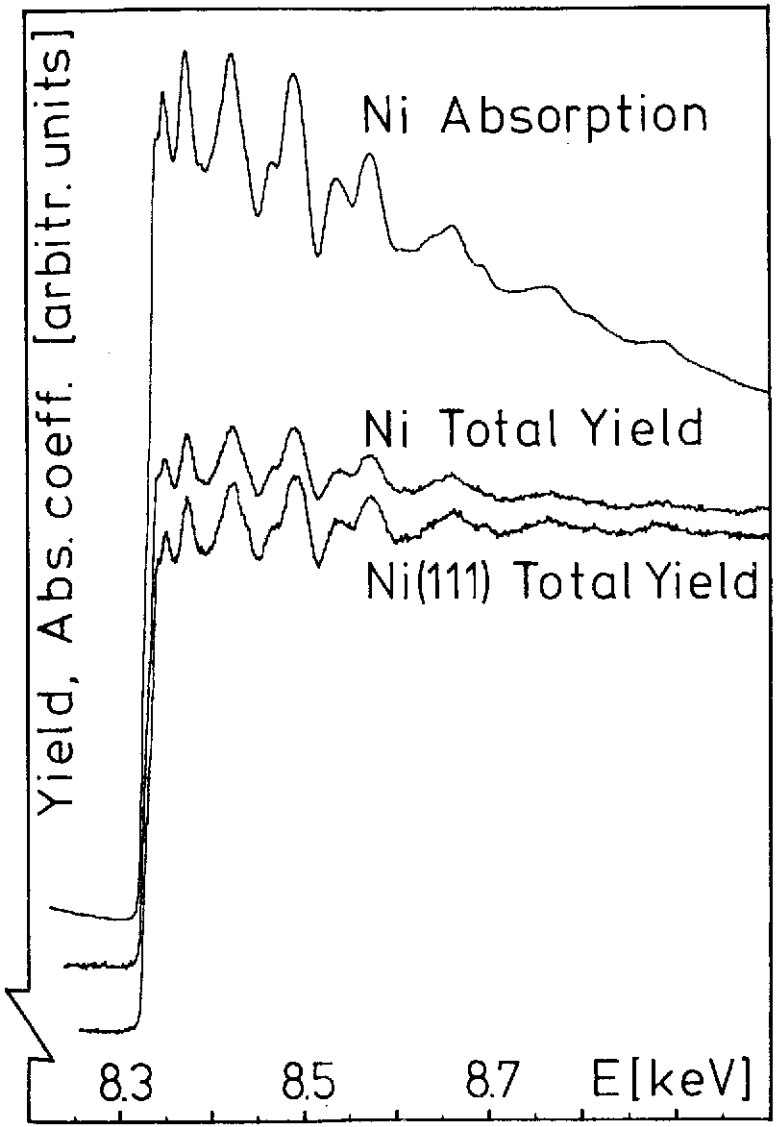
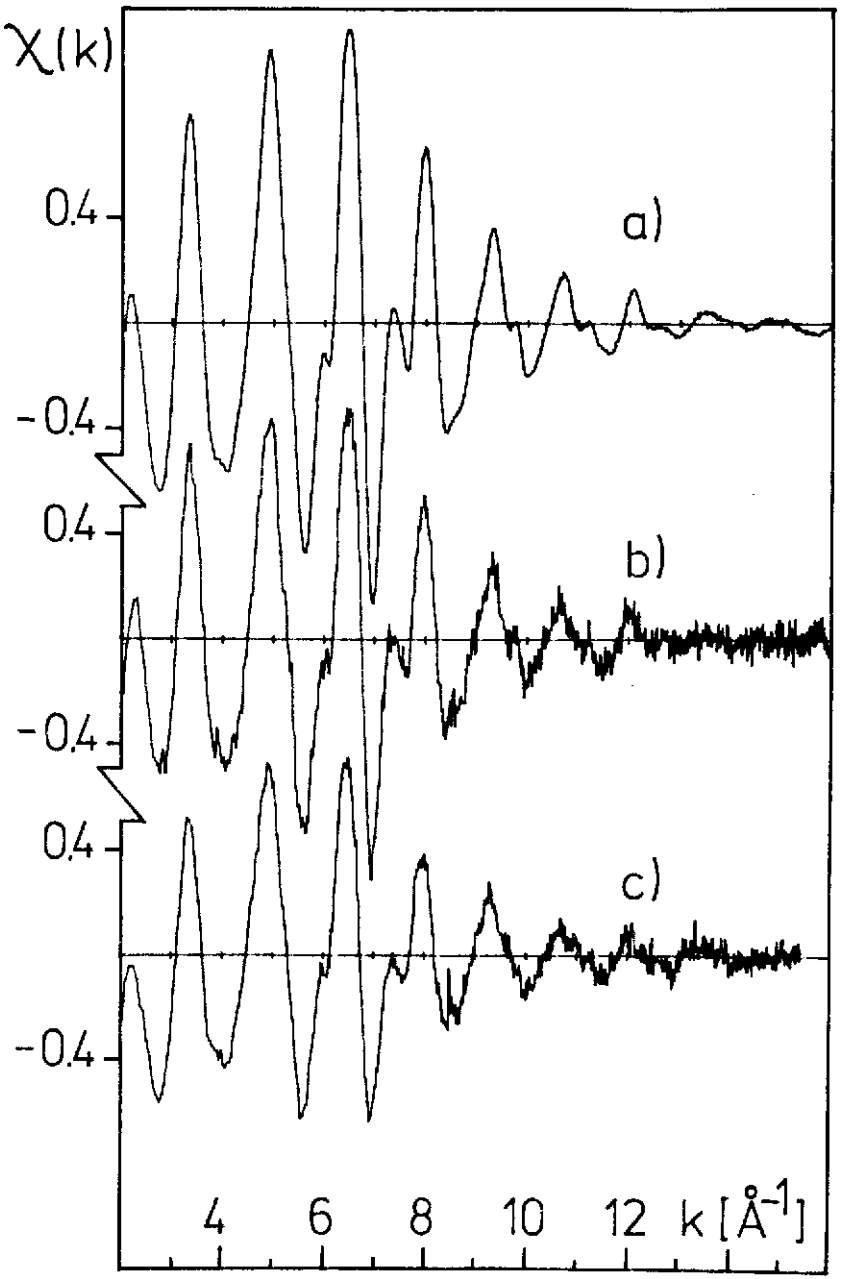

Yield, Abs. coeff. [arbitr. units]
Ni Absorption
Ni Total Yield
Ni(111) Total Yield
8.3
8.5
8.7
E[keV]

Fig. 2


χ(k)
0.4
-0.4
a)
0.4
-0.4
b)
0.4
-0.4
c)
4
6
8
10
12
k [Å$^{-1}$]

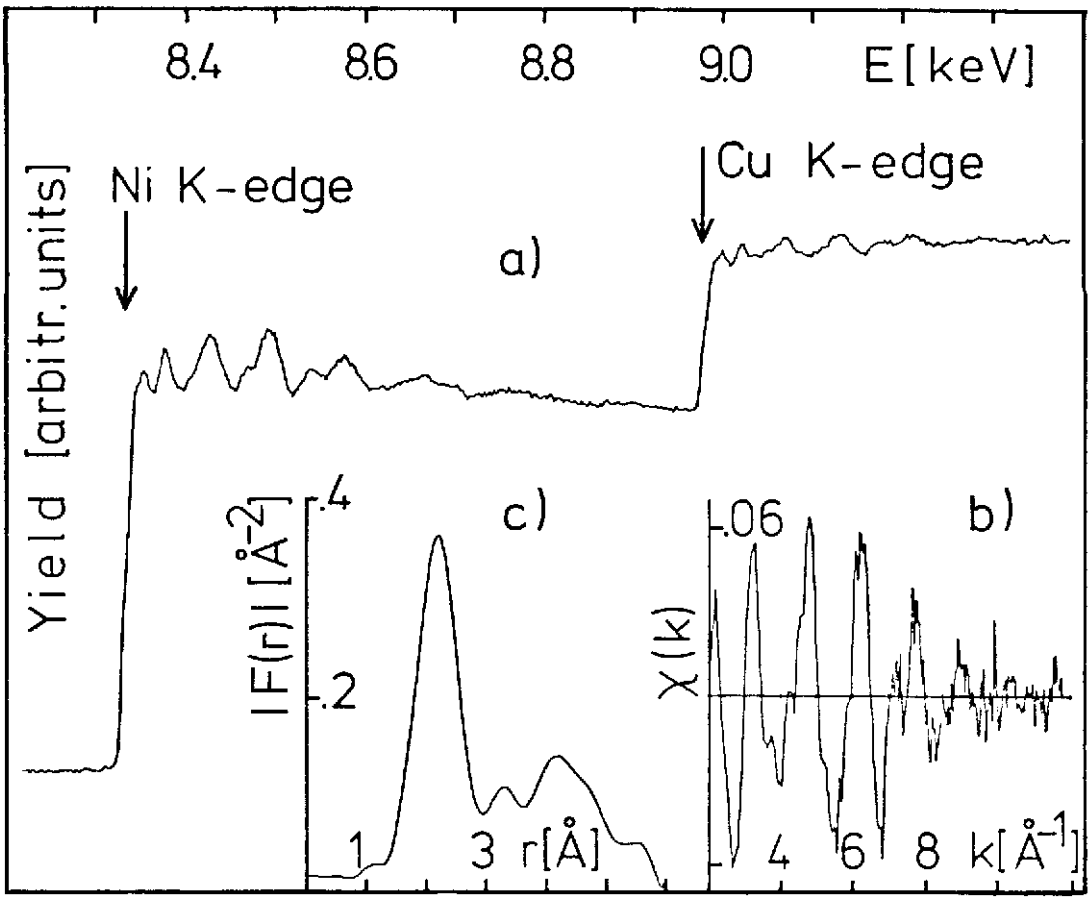

8.4
8.6
8.8
9.0
E[keV]
Ni K-edge
Cu K-edge
a)
Yield [arbitr.units]
c)
|F(r)| [Å$^{-2}$]
.4
.2
1
3 r[Å]
b)
.06
χ(k)
4
6
8 k[Å$^{-1}$]

Fig. 3

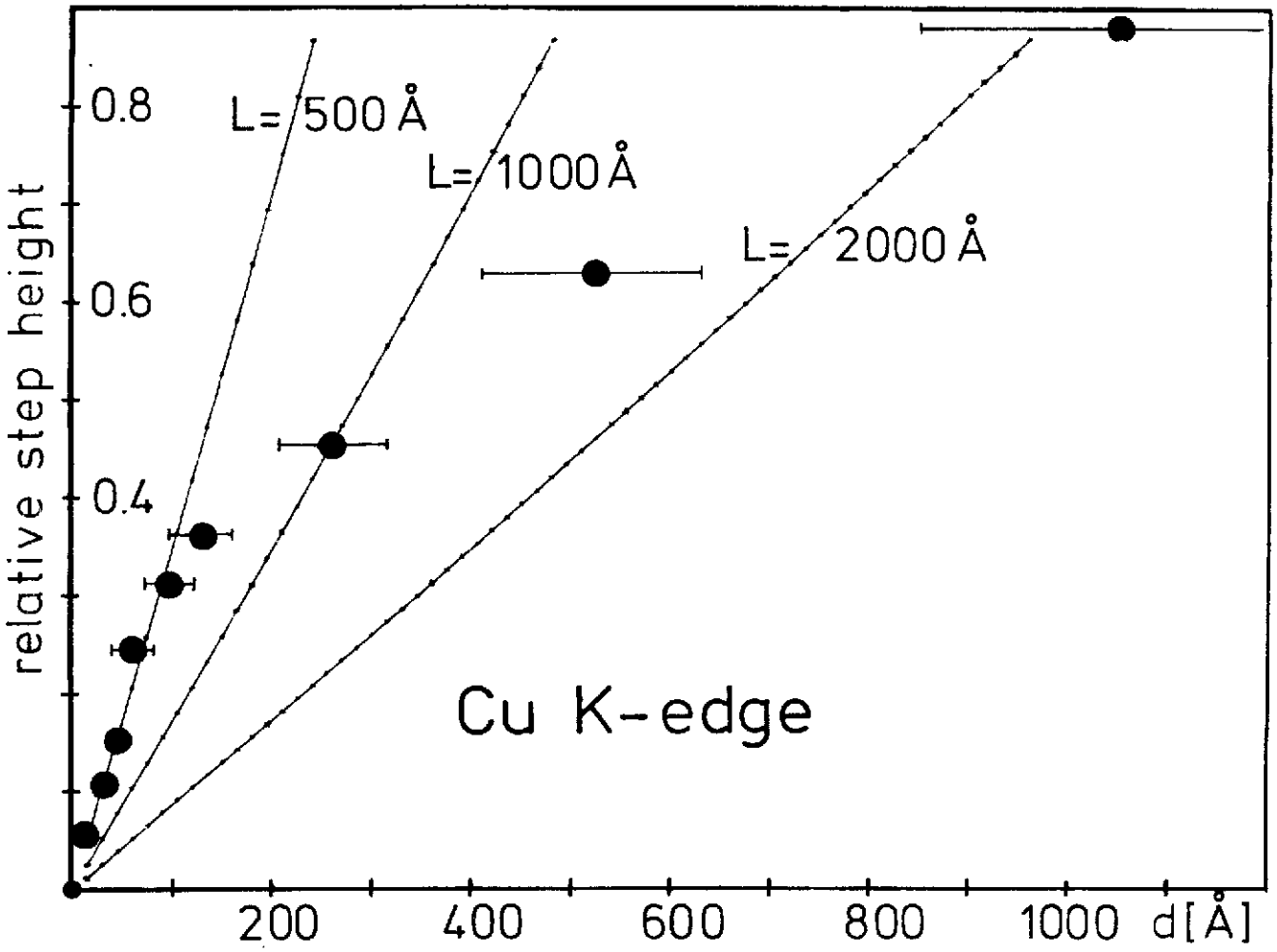

0.8
0.6
0.4
relative step height
L= 500 Å
L= 1000 Å
L= 2000 Å
Cu K-edge
200
400
600
800
1000
d[Å]

Fig. 4