

Modification of Photoelectron Spectra by Lattice and Spin Disorder

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Abstract

We present a new, unified model describing the influence of the temperature-induced lattice and the spin disorder on the angle resolved photoelectron spectra (ARPES); we also test this model by analysing the temperature evolution of the line shape for ARPES obtained at Cu(110), Ni(110), and Ni(111) surfaces, using the synchrotron radiation of BESSY

The thermally excited lattice vibrations cause noticeable changes in the angle resolved photoelectron spectra (ARPES), i.e., an increase in the linewidth, a shift in the line position, a decrease of the line intensity and a corresponding increase in the background is observed when the temperature is increased. An example is shown in Fig. 1. In the case of magnetic materials, characteristic changes of specific ARPES lines are produced in addition by thermally excited spin waves.

Considerable effort has been expended to understand the modifications in ARPES induced by the lattice vibrations. A good review of the subject can be found in the paper by White *et al* [1] and in the references cited therein. However, important problems remain to be solved, e.g., describing the variations of the intensity and the width of the ARPES line within the same model, separating the quasielastic and inelastic background from the elastic line, and also treating the influence of the spin waves on the same footing. In this paper, we describe the salient features of a new, unified model which allows to attack these problems. A more complete account will be given in a subsequent paper.

The temperature dependence of the ARPES line intensity can be described by a Debye–Waller factor [2], with the relevant momentum transfer commonly associated with the g vector of the direct optical transition [3], i.e., this model tries to describe the influence of the lattice vibrations by the phonon assisted indirect optical transitions. As a second order processes such an indirect transition has a much smaller transition probability than a direct transition. The indirect transitions can be identified in the optical spectra only in semiconductors below the gap where there are no direct transitions.

Although this model describes the temperature dependence of the ARPES line intensity, there are considerable difficulties to incorporate the increase of the line width with increasing temperature: The width of the elastic line does not change. It is true that the intensity of the indirect transitions increases as the wave vector g of the phonons approaches zero [1, 3], but their energy goes to zero as well which makes it difficult or even impossible to separate the direct from the indirect transitions in this limit.

We propose to solve this problem by considering the com-

bined effect of all thermally excited phonons on one particular electron excitation. Assuming the Born–Oppenheimer approximation to be valid for the optical transition we envisage a quasistatic strain of a particular magnitude and symmetry in a region large enough to define a local band structure. The bands of this local band structure will be shifted compared to those of the unstrained crystal, with the shifts proportional to the components of the strain tensor and the relevant deformation potentials. At a given instant of time, the local band structures will be different for different points in the crystal, and also at the same point for different times.

The elastic ARPES line at elevated temperature is thus broadened since it is the superposition of the direct transition contributions in the various local band structures. As in the case of X-ray photoemission [4], we model this broadening by convoluting the low temperature ARPES line with a Gaussian. However, our model suggests that the width of this Gaussian should be proportional to the average strain produced by all the phonons excited at the temperature considered, i.e. it should be possible to describe the temperature dependence of the line width by the average deformation potential of the relevant direct transition.

We further assume that the decrease in the intensity of the direct transition line broadened as described above and also the increase of the background with increasing temperature comes about by electron phonon scattering of the excited electrons. Thus the elastic line composed of the various contributions from the direct transitions in the different local band structures is attenuated as usual by a Debye–Waller factor with the provision that no definite momentum transfer can be identified because of the multiple scattering nature of the final state.

We test our model by analysing the temperature evolution of the line shape for ARPES obtained at Cu(110), Ni(110), and Ni(111) surfaces, using the synchrotron radiation of BESSY, polarised perpendicular to the (1 $\bar{1}$ 0) plane of detection. The photon energies $\hbar\omega$ (8.5 to 17 eV) and the angles of emission are selected to produce spectra which show the exchange doublet at low temperatures for the Ni surfaces. The respective energy and angle resolution is between 40 and 90 meV, depending on $\hbar\omega$ and the sample investigated, and 2° fwhm. The temperature ranges from 100 to 700 K, i.e., far below and well above the Curie temperature $T_c = 630$ K of Ni.

In the case of the Cu(110) spectra, the ARPES is dominated by the S_4 line, with a weak contribution of the S_2 line at lower binding energy which is symmetry forbidden in the nonrelativistic limit. Two spectra are shown in Fig. 1 for $T = 155$ K and 668 K. We obtain an excellent fit of the line

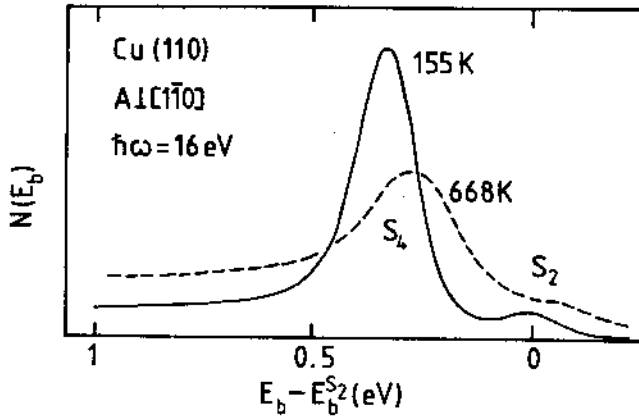


Fig. 1. Normal emission Cu(110) ARPES with the synchrotron radiation polarized along $[110]$ for two different temperatures.

shape at all temperatures by convoluting the spectrum obtained at the lowest temperature with a Gaussian. As expected from our model, the width parameter σ_u of this Gaussian which we determine by the least squares fit procedure is proportional to the average strain amplitude $\sqrt{\langle u^2 \rangle}$ for the temperature under consideration, calculated using the Debye model. Figure 2 gives an example, with $\sigma_r = 45$ meV describing the resolution of our spectrometer. Except for the small energy shifts which are also present, the evolution of the line shape with temperature is thus completely described by the average deformation potential of the S_4 transition.

In the magnetic case, we replace the actual spin disorder originating from thermally excited spin waves by a Maxwell distribution of spin spirals, characterized by the average wave vector q of these spirals. The scattering of electrons by such a spin configuration can be calculated analytically [5]. Aside from the lattice disorder which is treated as outlined above, the complicated temperature dependence of the Ni line shape is governed by q only, with $2\pi = (12.5 \pm 1.5)/\text{\AA}$ above T_c ,

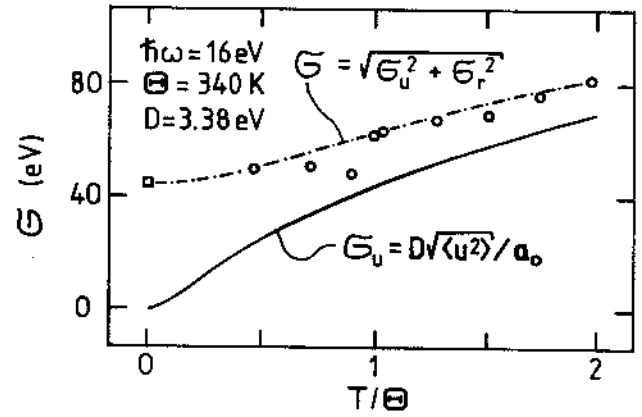


Fig. 2. Temperature dependence of the Gaussian with parameter σ as determined by the least squares fit procedure (dots) and as calculated by our model (dash-dotted) which assumes the temperature dependent σ_u to be proportional to the average lattice amplitude $\sqrt{\langle u^2 \rangle}$ calculated in the Debye approximation. The width parameter σ_r refers to the resolution of our spectrometer.

independent of the various different transitions involved. This shows that a considerable short range magnetic order persists above T_c .

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