Charge density waves and radiative transitions in sodium and potassium

Yu. M. Kobzar' and N. N. Bodnar
G. V. Karpenko Physicomechanical Institute, L'vov

(Submitted 24 January 1990)
Pis'ma Zh. Eksp. Teor. Fiz. **52**, No. 1, 686–690 (10 July 1990)

Several structural features have been observed in the emission spectrum of sodium and potassium as a result of a bombardment with slow electrons. The effect of temperature (293–4.2 K) on the emission characteristics were studied. The results are explained in terms of the recombination radiation of nonequilibrium carriers in the energy superstructure created by the charge density waves.

Despite extensive experimental studies, the electronic structure of ordinary metals continues to attract attention because many effects in the energy structure are yet to be discovered. The presence of superstructure in the conduction electron spectrum and the location of the lower limit of the interband transitions, for example, have not yet been determined unambiguously.[1–3]

To determine the energy structure of sodium and potassium near the intrinsic and lower interband absorption edge, we used an electron–photon spectroscopic method[4,5] which involved bombarding a metal with a slow electron beam and studying the characteristic features of the generated emission. Studies in the ultraviolet region using this method came to be known as the isochromatic bremsstrahlung spectroscopy or inverse photoemission.[6] Research in the IR region of the spectrum has made it possible to determine the radiative relaxation of the steady equilibrium distribution of electrons near the Fermi level.

The experiments were carried out in a superhigh vacuum chamber, $P_{\text{res}} \sim 7 \times 10^{-8}$ Pa. The Na and K films of 99.99% purity were deposited on a copper substrate by thermal evaporation from a quartz crucible. They were then bombarded

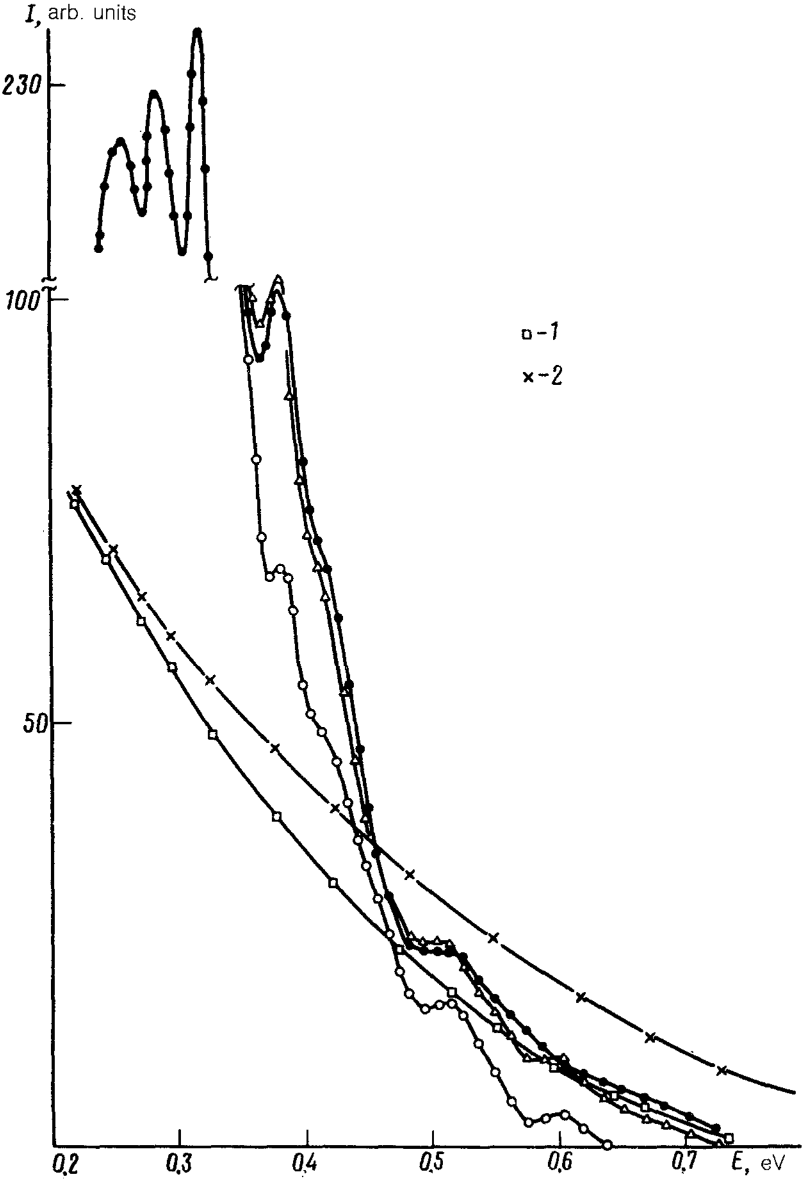

FIG. 1. Electron-photon emission spectrum for Na. ●—293 K; △—77 K; ○—4.2 K.

by an electron beam with an energy of 80–1600 eV and current density of 0.5–1.5 A/cm^2. The substrate was attached to a Dewar vessel, allowing us to cool the Na and K films to 4.2 K. The radiation from the chamber was transmitted through a sapphire window and directed to a high-transmission IR spectrometer with mirror optics. The radiation was detected by a receiver of threshold flux of PbS radiation (295 K and 77 K) and InSb radiation (77 K) in a synchronous detection mode with data acquisition on a minicomputer.

Figures 1 and 2 show the spectra of electron–photon Na and K emission at

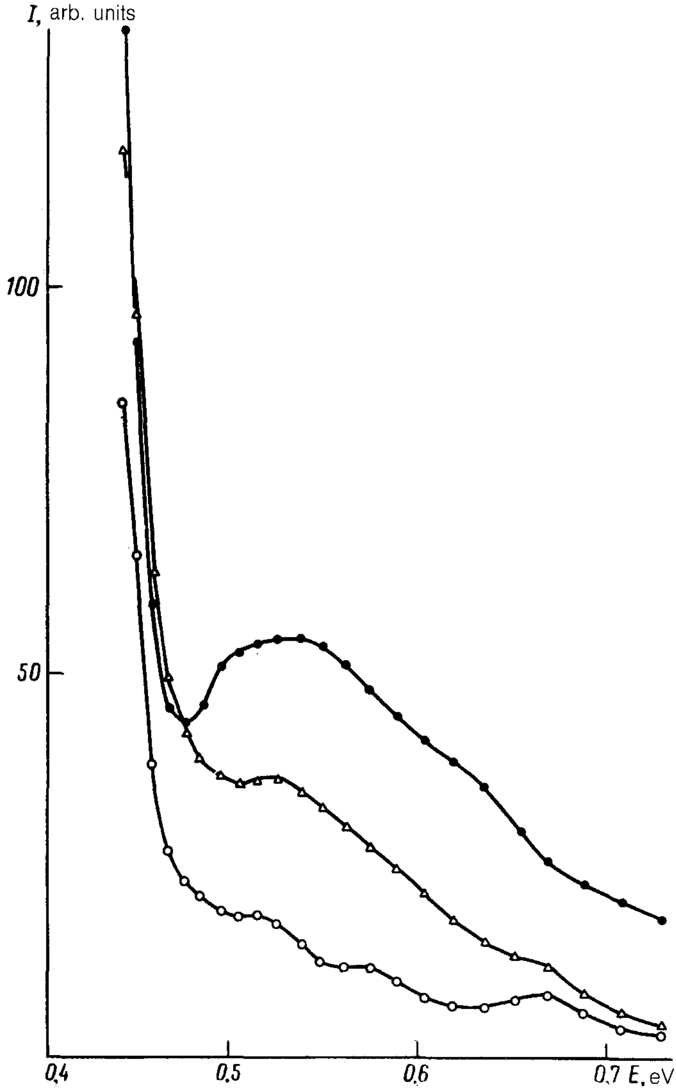

FIG. 2. Electron-photon emission spectrum. ●—293 K; ▲—77 K; O—4.2 K.

temperatures of 295, 77, and 4.2 K of the substrate. The shape of the emission spectrum can be explained in terms of two channels of radiative relaxation of nonequilibrium electrons, the first of which corresponds to the intraband transitions. To characterize the state of these electrons, we introduce the effective electron temperature Q_e.[7] Curves *1* and *2* in Fig. 1 show the results of calculation of the spectra of the indirect

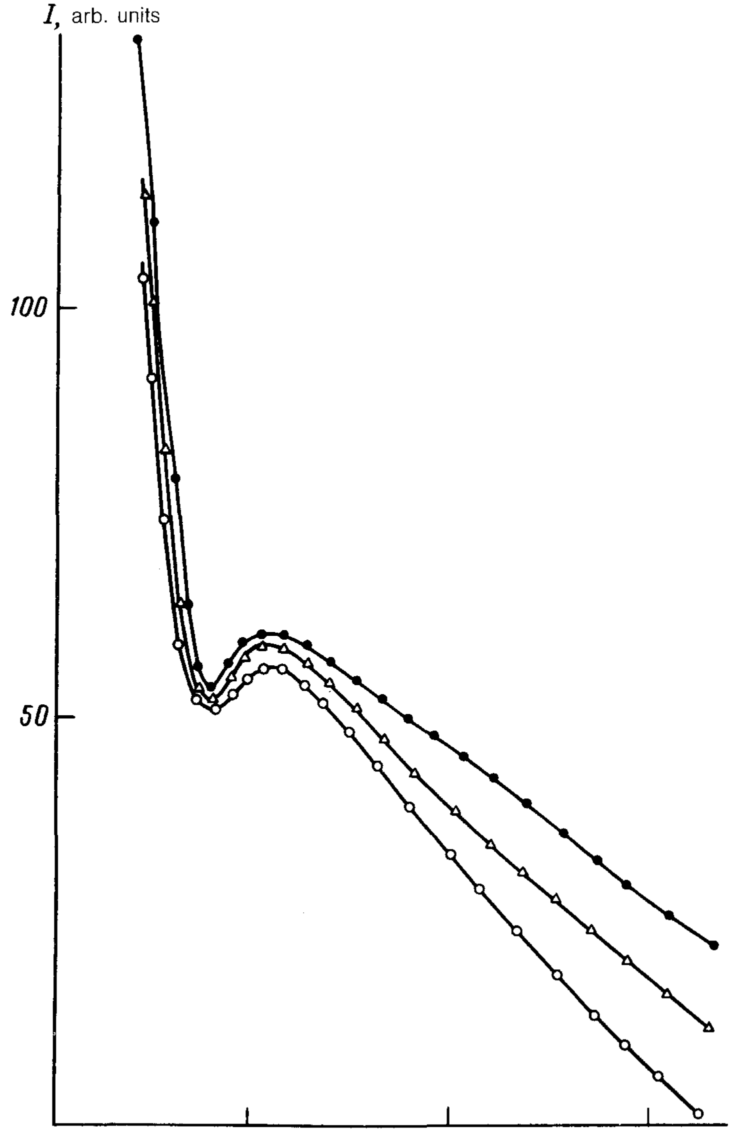

FIG. 3. Energy dependence of the electron-photon emission spectrum for Na. ●—1600 eV; ▲—1000 eV; O—800 eV.

intraband transitions of Na at $Q_e = 0.2$ and 0.4 eV. These curves describe to some degree the increase of the intensity with decreasing photon energy, especially down to 0.48 eV. On the other hand, the experimental spectra exhibit many structural features caused by the second relaxation channel of nonequilibrium electrons: the interband radiative transitions which occur as a result of the presence of the energy gaps in the electron dispersion near the Fermi level. The lower boundary of the interband transitions in the principal lattice is determined by the points at which the Fermi level crosses the planes of the first Brillouin zone. According to the estimates of Ref. 8, in the case of Na this characteristic feature corresponds to 0.46 eV. In our experiment the feature at $E_2 = 0.512$ eV probably corresponds to the lower boundary. This characteristic feature is attributable to the direct interband transitions, since the temperature has virtually no effect on it and it manifests itself clearly at all bombarding electron energies (Fig. 3).

Potassium also has a structural feature at $E_2 = 0.52$ eV, but the indirect transitions involving photons, in addition to the direct interband transitions, like those in Na, in this case play a dominant role, which accounts for the displacement of E_2 and the broadening of this special feature upon a change in temperature. The electron–photon emission spectra for sodium and potassium upon lowering the temperature of the metal, especially down to 4.2 K, exhibit a series of special features at $E_3 = 0.58$ eV and $E_4 = 0.67$ eV for potassium and at $E_0 = 0.25$ eV, $E_1 = 0.293$ eV, and $E_3 = 0.605$ eV for sodium. These features are probably traceable to the many-particle interaction potential. Some of the more obvious features are the lattice instabilities produced as a result of interaction of the electrons and photons with the wave vector $\mathbf{k} = 2\mathbf{k}_F$. An example of such an instability are the charge density waves (CDW). The potential of the charge density waves $V_{\rm CDW} = 2\alpha\cos(\mathbf{Q}\cdot\mathbf{r})$, where α is the amplitude, and $\mathbf{Q}$ is the wave vector of the CDW, leads to the appearance of energy gaps in the electron spectrum near the Fermi level.[2] The radiative transitions occur between the zones that are formed. The photon energy in this case is 2α, i.e., twice the CDW potential for the given direction in the crystal. A comparison of simplified calculations of the position of the CDW-induced structural features in the absorption spectra of Na and K,[2] with our experimental data shows that there is a factor of two difference for the structural features at photon energies below 0.3 eV.

[1] A. J. Sievers, Phys. Rev. B **22**, 1600 (1980).
[2] F. E. Fragachan and A. W. Overhauser, Phys. Rev. B **31**, 4802 (1985).
[3] I. R. Collins *et al.*, J. Phys. C: Sol. St. Phys. **21**, L655 (1988).
[4] Yu. M. Kobzar' *et al.*, Fiz. Tverd. Tela (Leningrad) **28**, 3500 (1986) [Sov. Phys. Solid State **28**, 1969 (1986)].
[5] Yu. M. Kobzar' *et al.*, Pis'ma Zh. Eksp. Teor. Fiz. **50**, 323 (1989) [JETP Lett. **50**, 358 (1989)].
[6] J. B. Pendry, J. Phys. C: Sol. St. Phys. **14**, 1381 (1981).
[7] Yu. M. Kobzar' *et al.*, Ukr. Fiz. Zh. **33**, 207 (1988).

Translated by S. J. Amoretty