

# A Study of Fermi Surfaces of the $\beta$ -Phase Cu-Ge and Cu-Si Alloys by Positron Annihilation(Physics)

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### Crystal Structures of Pyroxene-Type $\text{ZnSiO}_3$ and $\text{ZnMgSi}_2\text{O}_6$

N. MORIMOTO, Y. NAKAJIMA, Y. SYONO, S. AKIMOTO and Y. MATSUI  
Acta Crystallogr., **B31** (1975), 1041.

The crystal structures of two pyroxene polymorphs of  $\text{ZnSiO}_3$ , and the orthopyroxene of  $\text{ZnMgSi}_2\text{O}_6$  have been studied. The monoclinic  $\text{ZnSiO}_3$  crystallizes in the space group  $C2/c$  with  $a=9.787$ ,  $b=9.161$ ,  $c=5.296\text{\AA}$ ,  $\beta=111.42^\circ$ ,  $Z=8$ ; orthorhombic  $\text{ZnSiO}_3$ ,  $Pbca$ ,  $a=18.204$ ,  $b=9.087$ ,  $c=5.278\text{\AA}$ ,  $Z=16$  and orthorhombic  $\text{ZnMgSi}_2\text{O}_6$ ,  $a=18.201$ ,  $b=8.916$ ,  $c=5.209\text{\AA}$ ,  $Z=16$ . In the structure of the monoclinic  $\text{ZnSiO}_3$ , Zn atoms are coordinated octahedrally (at M1 sites) and tetrahedrally (at M2 sites). The Zn atoms at the M2 sites are not coordinated by the bridging oxygen [O(3)] of the  $\text{SiO}_3$  chains. In the orthorhombic  $\text{ZnSiO}_3$ , however, Zn atoms at the M2 sites have an irregular octahedral coordination including O(3) atoms. Because of the difference in coordination of O(3) to Zn atoms, the shape of the  $\text{SiO}_3$  chains in the two polymorphs of  $\text{ZnSiO}_3$  is different. The structure of the orthorhombic  $\text{ZnMgSi}_2\text{O}_6$  is intermediate between that of enstatite ( $\text{MgSiO}_3$ ) and the orthorhombic  $\text{ZnSiO}_3$ . Zn atoms are partially ordered in M1 and M2 sites with site occupancies of 36 and 64% respectively.

### Electrical Resistivity of Laves Phase Compounds Containing Transition Elements. I. $\text{Fe}_2\text{A}$ (A=Sc, Y, Ti, Zr, Hf, Nb, and Ta)

Kôki IKEDA and Takurô NAKAMICHI  
J. Phys. Soc. Japan, **39** (1975), 963.

The electrical resistivity of a series of  $\text{Fe}_2\text{A}$  Laves phase compounds was measured in order to investigate its mutual correlation with their magnetic properties. In the ferromagnetic or antiferromagnetic  $\text{Fe}_2\text{A}$  compounds (A=Sc, Y, Ti, Zr, Hf, and U), a linear relation between the magnetic resistivity at temperatures above the Curie or Néel point and the localized magnetic moment was found, which means that the magnetic resistivity of these compounds is governed by the magnitude of magnetic moments. The electrical resistivity in the Pauli-paramagnetic  $\text{Fe}_{2+x}\text{Nb}_{1-x}$  and  $\text{Fe}_{2+x}\text{Ta}_{1-x}$  compounds with  $x \approx 0$  shows a fairly large temperature variation, which seems to be due to the paramagnon scattering, whereas  $\rho$ - $T$  curves in the iron-rich compounds suggest that the appearance of ferromagnetism is caused by the existence of the excess iron atoms occupying the wrong atomic sites.

### A Study of Fermi Surfaces of the $\alpha$ -Phase Cu-Ge and Cu-Si Alloys by Positron Annihilation

Toshiharu SUZUKI, Masayuki HASEGAWA and Makoto HIRABAYASHI  
Appl. Phys., **5** (1974), 269.

Angular correlation measurements on the fcc solid solutions of Cu-Ge and

Cu-Si alloys have been carried out on single crystals with four crystallographic orientations by a crossed-slit geometry. The results on both the alloys are nearly the same. The  $\langle 111 \rangle$ -neck radius and the  $\langle 100 \rangle$ -radius of the Fermi surfaces increase almost linearly with increasing electron concentration in accord with previous results on Cu-Al and Cu-Zn alloys. The Fermi surface does not touch the square faces of the Brillouin zone at the solubility limit. The results agree fairly well with a calculation based on the sinking-conduction band model.

### Chemistry

#### **On the Surface Chemical Reactions of Metal and Oxide XPS Samples at 300-400° at a High Vacuum Produced by Oil Diffusion Pumps**

Kichinosuke HIROKAWA, Fumihiro HONDA and Masaoki OKU

J. Electron Spectrosc. & Relat. Phenom., 6 (1975), 333.

Metal and oxide surface reactions formed by heating in the spectrometer at 300–400° at a vacuum of ca.  $10^{-9}$  Torr (oil diffusion pumps) were studied. As a result of spectral observations before and after heating, the metals studied were classified into five groups. In the first group, oxide films on the metal surface are easily evaporated because of the high vapour pressure of oxide; in the second, the oxide films are easily reduced in the spectrometer; in the third, the oxide film formed on the metal is reduced but the bulk oxide is not easily reduced; in the fourth, very stable oxide films are formed and the bulk oxide is also stable; and finally in the fifth, the oxide film formed on the metal is apparently reduced, yet the bulk oxide is very stable.

#### **Photoelectron Spectral Intensities of Some First Transition Series Elements in Metal Cyanides Containing Inequivalent Atoms**

Masaoki OKU, Kichinosuke HIROKAWA and Shigero IKEDA

J. Electron Spectrosc. & Relat. Phenom., 6 (1975), 451.

Photoelectron spectral intensities of some first transition series elements were studied for metal cyanides containing inequivalent atoms. The spectra of low-spin ions coordinated via carbon to the cyanide ion, and of high-spin ions coordinated through nitrogen were separately obtained from manganese, iron, and cobalt cyanides. Metal 2p spectra obtained as sums of the appropriate spectra of low- and high-spin ions were nearly coincident with the spectra of the compounds containing inequivalent atoms. These results show that the intensity of the 2p electron for each atom must include the main peak and perhaps multiplet splitting effects, shake-up effects, and the inelastic scattering tail, and verify the non-interaction nature of the inequivalent atoms in these compounds.