ELECTRONS AND PHONONS IN LAYERED CRYSTAL STRUCTURES

PHYSICS AND CHEMISTRY OF MATERIALS WITH LAYERED STRUCTURES

VOLUME 3

ELECTRONS AND PHONONS IN LAYERED CRYSTAL STRUCTURES

Edited by

T. J. WIETING

U.S. Naval Research Laboratory, Washington, D.C. 20375, U.S.A.

and

M. SCHLÜTER

Bell Laboratories, Murray Hill, N.J. 07974, U.S.A.

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FOREWORD

This volume is devoted to the electron and phonon energy states of inorganic layered crystals. The distinctive feature of these low-dimensional materials is their easy mechanical cleavage along planes parallel to the layers. This feature implies that the chemical binding within each layer is much stronger than the binding between layers and that some, but not necessarily all, physical properties of layered crystals have two-dimensional character. In Wyckoff's *Crystal Structures*, SiC and related compounds are regarded as layered structures, because their atomic layers are alternately stacked according to the requirements of cubic and hexagonal close-packing. However, the uniform (tetrahedral) coordination of the atoms in these compounds excludes the kind of structural anisotropy that is fundamental to the materials discussed in this volume. An individual layer of a layered crystal may be composed of either a single sheet of atoms, as in graphite, or a set of up to five atomic sheets, as in Bi_2Te_3. A layer may also have more complicated arrangements of the atoms, as we find for example in Sb_2S_3. But the unique feature common to all these materials is the structural anisotropy, which directly affects their electronic and vibrational properties.

The nature of the weak interlayer coupling is not very well understood, despite the frequent attribution of the coupling in the literature to van der Waals forces. Two main facts, however, have emerged from all studies. The first is the extraordinary variation in the interlayer coupling strength from material to material. By comparison with the forces acting within the layers, the interlayer forces are smaller by factors ranging between twenty and a thousand. These ratios have been determined from phonon studies, and their values are a convenient measure of the structural anisotropy of a particular material. The second fact is the nearly three-dimensional character of certain electronic energy states in materials that otherwise show large structural anisotropy. This combination of two- and three-dimensional effects in the same material is an intriguing aspect of the physical properties of layered solids. Since most studies have focussed on the stronger intralayer forces, few quantitative models of the interlayer interaction have thus far been proposed, and much important work remains to be done in this area.

In organizing this review the editors have chosen to restrict the number of contributions, so that a broader and more synthetic treatment of electron and phonon energy states could be achieved. The first three articles in this volume, contributed by Schlüter and Fong, review the calculations of energy bands in layered materials and the supporting optical data. After discussing the group theoretical tools, the authors consider the various theoretical methods used to calculate the band structures of layered crystals. They then discuss specific materials and their bonding models and

compare theoretical results with relevant experiments. The two articles on phonons, which make up the second part of the volume, divide along the lines of the experimental techniques employed in studying lattice vibrations. Long-wavelength phonons are treated in the article by Wieting and Verble on infrared absorption and Raman scattering, and phonon dispersion is taken up in the article by Wakabayashi and Nicklow on inelastic neutron scattering. Each article in turn attempts to evaluate all the published work on electron or phonon energy states in inorganic layered crystals.

In a rapidly growing field of research, the most recent results are inevitably omitted from consideration. Since completing the manuscript, a number of papers have appeared that supplement the discussion in this review or provide examples of new families of layered crystals, or in some cases describe novel physical effects. Perhaps the most interesting recent development is the discovery of electron charge density waves in the tantalum dichalcogenides and the periodic structural distortions that are associated with the formation of these waves. Many investigators have already entered into this new area. An assessment of this and other work, however, must remain for future reviews of electrons and phonons in layered crystals.

U.S. Naval Research Laboratory T. J. WIETING AND M. SCHLÜTER
Bell Laboratories
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