Theories of metallic behavior — Roadmaps to reality

Groups of researchers within the Division of Physics shape theory to reality in describing fundamental physical properties of metals.

Physics is wedded to theory. An important role of any physicist is to derive theoretical models which give a clear mathematical description of the physical laws by which matter behaves, intellectual templates which duplicate the mechanics of nature.

The test of any true theory lies in its accuracy and predictive strength; observable properties of the physical world must be predicted *a priori* from the derived model.

Groups of researchers within the National Research Council's Division of Physics are working at this interface between theory and reality to study different aspects of metallic behavior.

For example, metal physicists describe common physical properties of metals such as malleability or conductivity at the fundamental level of atomic theory.

Any metal crystal can be visualized as a regular, close-packed aggregate (lattice) of positively-charged atoms bound together by a sea of electrons. Unlike the situation with common covalent bonds, the binding electrons are not localized between atoms, but, rather, are shared by the entire crystal. The outermost electrons, which are weakly bound to the lattice, have a maximum energy called the Fermi level; this value is characteristic for each metal. These highest energy electrons are responsible for many of a metal's electrical and magnetic properties.

Researchers in the Metal Physics Section study these electrons through a form of atomic "mapping" by low temperature, de Haas-van Alphen (dHvA) experiments, in which single crystals of a metal are studied in a strong magnetic field. Much like the meteorologist who joins map readings of equal pressure into isobars, the metal physicist can construct a "Fermi surface" for each metal by mapping regions of constant electron energy on a three-dimensional momentum diagram.

In the simplest case, where the outermost electrons do not interact strongly with the lattice, the resulting Fermi surface is spherical. However, for most metals, the electrons' motion is affected by the lattice, and Fermi surfaces of uneven contour are obtained. Their topology corresponds to peaks and valleys of electron momentum.

"A thorough knowledge of Fermi surfaces provides an invaluable profile of electronic structure," explains Dr. Ian Templeton. "Recently, we have developed a new technique to examine both pure metals and alloys with unprecedented precision. In the latter cases, changes in the electronic properties of metals accompany alloying, and affect the shape and size of the Fermi surface."

The same conduction electrons described by the Fermi surface are also responsible for the important property of electrical conductivity in metals, an object of study in the High Temperature Physics Section.

For conducting materials such as copper, electrons can move freely through the lattice, transferring electrical charge as they do so. In an insulator, however, these electrons are bound tightly to the atoms.

Using this model, scientists in the past have tried, with limited success, to explain another metallic property, thermal conductivity or the transport of heat. The correspondence between thermal and electrical conductivity has been tempting since the main transport agents in both cases are the metal's valence electrons.

By studying the transport properties of metals at high temperatures, NRC physicists hope to piece together a more rigorous theoretical model of thermal conductivity. Eventually, by finding the elusive link between thermal and electrical conductivity theories, scientists may make predictions of one through their knowledge of the other.

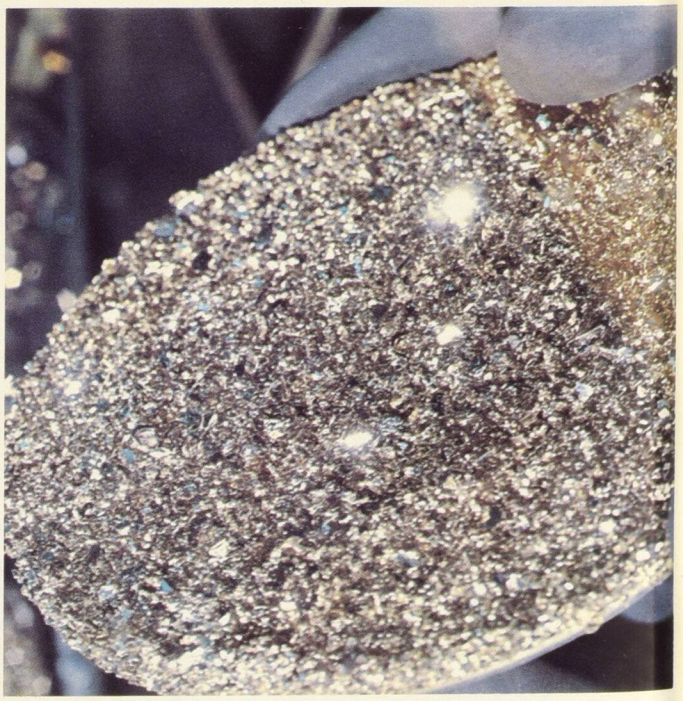
The High Temperature Physics Section is one of the few in the world able to measure thermal conductivity accurately over the temperature range 80 - 1 250°K (−193 − +977°C).

"Although our work is of a fundamental nature," says Dr. Marek Laubitz, "applications may follow with the increasing precision of thermal engineering. For example, predictions of heat transfer characteristics of metals at high temperatures are becoming an important aspect in the efficient extraction of heat from nuclear reactors."

Analogous to the role played by electrons in determining the conductivity properties of metals is that played by so-called dislocations in determining the mechanical properties. Almost any pure metal is soft and malleable because its crystals are made up of sheets of atoms arranged in parallel layers like playing cards in a deck. The assembly, like the deck, can deform easily as the crystal planes (similarly the cards) slip over one another. However, planes of atoms do not slide simultaneously over their whole area, but rather a boundary (called a dislocation line) between the slipped and unslipped regions of the atom plane, moves through the crystal.

The mechanical properties of metals depend on the ease with which dislocations can move. In a very pure metal which has been heated to high temperatures and then cooled, there are few obstacles to hinder dislocation motion and the material is soft and malleable.

Such metals can be made stronger by introducing obsta-



In studying high temperature thermal conductivity, physicists require metal specimens of consummate purity. These crystals of strontium were grown in an insulated container under an atmosphere of dry helium gas.

Pour étudier la conductivité thermique à haute température, les physiciens ont besoin d'échantillons de métaux de grande pureté. Ces cristaux de strontium se sont développés dans une enceinte isolée sous une atmosphère d'hélium sec.