Pursuing a metals theory

Light cast on the structure of the alkali metals throws shadows on materials research

by Carl Behrens

Dr. Overhauser and a potassium sample: The simple metals are not so simple.

Scientists, following the dictum not to make more hypotheses than they need, like to keep their theoretical models simple. Unnecessary complications are not popular.

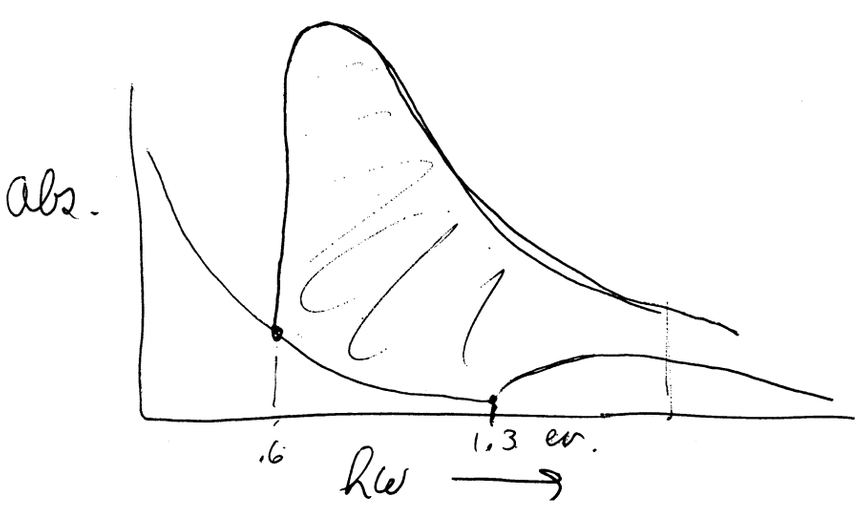
But when too many facts fall outside the model, it has to be expanded. The theoretical picture of sodium, potassium and other alkali metals has reached that point, says solid-state physicist Albert W. Overhauser, of the Scientific Laboratories at Ford Motor Co., who proposes a new, more complex model. If the new model is accurate, a tremendous body of theoretical work on the properties of metals will have to be revised.

Only in the last few decades has it been possible to describe the details of how atoms in a solid behave. Out of this understanding has come, among other technological advances, the development of transistors and other semiconducting devices.

Although the alkali metals are not as technologically useful in their pure state as other metals—they react too quickly with other elements—their simple atomic structure has made them basic to the understanding of other more complicated elements.

Their distinguishing feature is that they have only one, easily-detachable electron in the outer shell, and few electrons in inner shells. From this, it has appeared possible to assume that the outer electrons are free to move about within the solid, forming a sort of gas, instead of being tied down to orbits around particular atoms. As in other conducting metals, it is this gas of free electrons that carries electric current.

The simple model of the alkalis assumes that the sum of all forces on any one outer-shell electron is zero; that is, the forces cancel out, and the electrons move about unaffected, on average, by the atomic nuclei. A result of this is that the density of the electron gas is the same throughout the metal.



Sketch by Overhauser

Absorption of light by potassium shows unexpected peak at 0.6 electron volt.

From this simple model, the properties of the metals can be predicted. Physicists can measure what happens to the metals when they are bathed in light, placed in magnetic fields, or subjected to electric forces. Similar quantities can be measured for more complex elements, too—elements like copper, iron and chromium whose theoretical models are more complicated.

Differences in measured behavior of simple and complex metals can give clues as to the structure of those more complicated elements. In this way, the simple theory helps experimenters to choose what measurements to make, and the experiments elaborate the theory.

The trouble is, according to Dr. Overhauser, that experiments with alkali metals have turned up results different from those predicted by the simple model.

The amount of light energy, for instance, that is absorbed by a metal, compared with what it reflects, depends on the frequency of the incoming light. The absorption pattern of metals is a commonly measured quantity.

One of the most important misbehaviors of the alkali metals is the way they absorb light.

According to the simple theory, absorption by potassium should decrease smoothly with increasing frequency up to 1.3 electron volts. But an experiment four years ago in Germany showed a big peak in the absorption curve at 0.6 electron volt.

Other effects, mostly concerned with the magnetic behavior of the metals, have been observed to vary from what

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would be predicted by the simple model. The electrical resistance of alkali metals is seen to increase rapidly in a magnetic field, contrary to the theory; the amount it increases depends on the orientation of the metal crystals, and is sensitive to stress.

The latest anomaly observed is the tailing off of the Hall effect. When a strip of metal, carrying a current, is placed in a magnetic field, a voltage develops across the edges of the strip, perpendicular to the current flow and the field. This voltage, according to the simple model, is proportional to the current and the field; that is, the proportionality constant, called the Hall constant, doesn't change.

But with increasing magnetic fields above 50 kilogauss, the Hall constant has been observed to decrease in experiments on alkali metals at the Massachusetts Institute of Technology's Francis Bitter National Magnet Laboratory, reports Dr. P. A. Penz of the Ford Laboratories in the April 1 PHYSICAL REVIEW LETTERS.

In order to explain these and other unexpected results, says Dr. Overhauser, it is necessary to abandon the simplifying assumption that the electron gas has the same density everywhere.

Instead, he says, the electrons interact with each other to cause bunching, so that the density of electrons varies in a sort of washboard effect. This variation Dr. Overhauser calls a charge density wave.

If the charge density wave is cranked into the theoretical model, the behavior that has been observed in sodium and other alkali metals can be predicted, says Dr. Overhauser. But acceptance of the theory is slow.

One reason physicists have been reluctant to accept the charge density wave is that it complicates experiments as well as theories.

This is because the character of the wave can be changed by exterior conditions, such as magnetic fields. That means in turn that a lot of physical qualities that had been assumed constant actually change under varying conditions, and the very act of observing them could affect the value obtained. The Hall constant is an example of this.

One prediction that hasn't been observed as yet is that if electron behavior is modified, it should affect the arrangement of positive ions in the metal also.

Although the experiment would be difficult, requiring exceptionally sensitive measurements, it should be possible to observe that effect with a really careful search of X-ray diffraction patterns from single crystals.