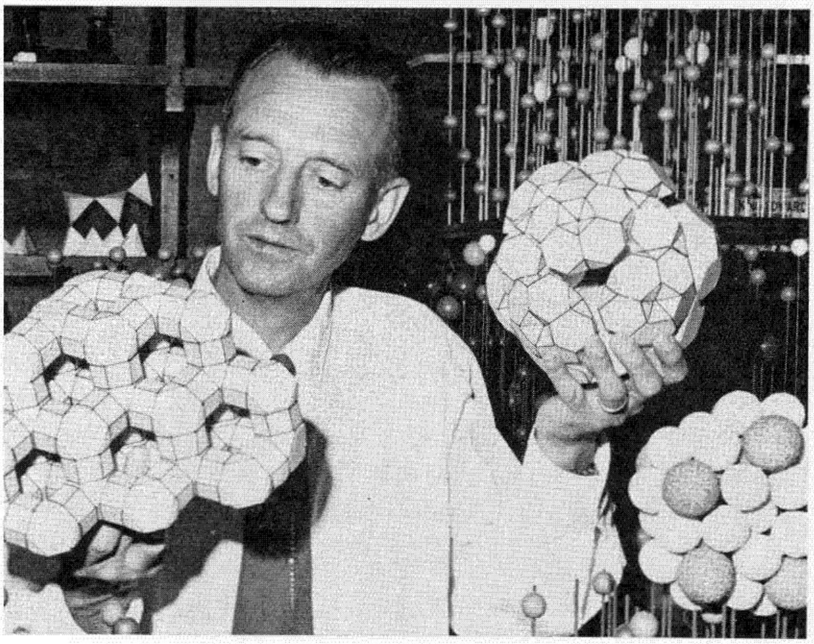

ATOMIC ARRANGEMENT

Dr. Sten Samson, senior research fellow in chemistry at Caltech, is making major contributions to metallurgy by investigating how the metal atoms in certain alloys organize themselves into geometric, flower-like patterns.

Dr. Samson and Dr. Linus Pauling, pioneer in this field, have received a $41,000 grant from the National Science Foundation, which is joining the Office of Naval Research in support of this work.

These complex structures of intermetallic compounds are of particular value because in them each kind of atom can be studied in many different environments. The distances reveal the atoms' bonding properties, and the forces that bind one atom to another are responsible for many physical properties of metals.

While the nature of the chemical bond in many substances is fairly well understood, considerable work has yet to be done to elucidate the nature of the metallic bond.

Dr. Samson recently made an important step forward in his field by determining the precise locations of all 1,192 atoms in the structural unit of an intermetallic compound of sodium and cadmium. This is the most complex inorganic compound to ever have its atomic arrangement determined. The job took more than a year, with Dr. Samson working up to 16 hours a day seven days a week.

The structural unit of the sodium-cadmium compound is a cube whose sides are less than one eight-millionth of an inch long. There are 1,192 atoms neatly packed inside it. The atoms are arranged in 8 identical sub-units of 144 atoms each. Each sub-unit, in turn, is composed of symmetrically arranged smaller units, which are polyhedral. The largest polyhedron consists of 12 of the smaller cadmium atoms and 4 of the larger sodium atoms forming a shell around one sodium atom.

It is the arrangement of the atoms in these polyhedra and the arrangement of the polyhedra with respect to one another in patterns like petals on a flower that may reveal many of the secrets of the properties of alloys.

Dr. Samson is now working on the structures of two other complex intermetallic compounds—one of copper and cadmium that contains about 1,116 atoms; and the other of magnesium and aluminum, whose unit structure is composed of about 1,200 atoms.

Precisely pinpointing the position of every atom in such a complex structural unit is a formidable task. There is no straightforward way of working out these complex structures. Intuition and educated guesses are necessary to determine the model of the structure. Subsequently, the correctness of the model must be verified by comparing calculated data with data that have been obtained by x-ray techniques.

Dr. Samson has simplified the problem of working out cubic metal structures with a special technique he developed. It makes use of all the symmetry represented in the structural unit. Transparent templates of sectioned polyhedra are fitted together on symmetry charts designed by Samson, like pieces of a puzzle. The charts then guide the search for a reasonable structural pattern, or motif.

"It is interesting to see how nature, even in this submicroscopic realm, insists on symmetry and beautiful geometric designs," says Dr. Samson. "Despite the complexity of these designs, there appears to be a striving for simplicity. Similar structural building blocks of atoms are used over and over again in a variety of combinations, leading to ever more complex-appearing structures."