

Semiconductors with Chalcopyrite Structure

It was recently reported¹ that certain compounds crystallizing with a triply substituted diamond lattice of the chalcopyrite type are semiconductors. We would report here optically determined energy gaps for a further four such compounds. These, together with the previously reported values for copper indium selenide and copper iron sulphide, are shown in Table 1.

Table 1

Material	Optical gap (eV.)	Material	Optical gap (eV.)
Cu In S ₂	1.2	Ag In Te ₂	0.96
Ag In Se ₂	1.18	Cu In Te ₂	0.95
Cu In Se ₂	0.92	Cu Fe S ₂	0.53

The copper iron sulphide was of mineral origin; all other materials were synthesized directly from the constituents in sealed evacuated silica tubes. A more detailed account of the work is being given elsewhere².

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¹ Goodman, C. H. L., and Douglas, R. W., *Physica*, **20**, 1107 (1954).

² Austin, I. G., Goodman, C. H. L., and Pengelly, A. E., *J. Electrochem. Soc.* (to be published).

Effects of Trace Elements on Embrittlement of Steels

IN the course of investigations to assess the factors controlling the embrittlement of steels, a wide variety of steels of commercial origin has been studied. It was found that the Charpy impact transition ranges of all the steels were raised—although to varying extents—if the steels were exposed at 450° C. for lengthy periods. In many instances the transition range still remained below room temperature after exposure at 450° C., and the steels were not, therefore, brittle at room temperature. Nevertheless, it was apparent that an embrittlement mechanism was operating at 450° C. in all the steels.

It has long been suspected that trace elements play an important part in the embrittlement of steels, and steels of high purity have therefore recently been studied. Although the programmes planned are still far from complete, the results already obtained are of sufficient interest to justify reporting.

A commercial 3 per cent nickel-chromium steel of the BS.En 23 type, when oil-quenched as $\frac{1}{8}$ -in. diameter bar from 840° C. followed by tempering at 625° C. and water-quenching, had a Charpy V-notch impact transition range extending from -35° to 150° C. After reheating the hardened and tempered steel at 450° C. for 168 hr. and water quenching, the impact transition range extended from 230° to 20° C.

A steel of the same nominal composition, carbon 0.30 per cent, nickel 3.0 per cent and chromium 0.75 per cent, was prepared from carbonyl iron powder and other pure raw materials in powder form

by compacting, sintering *in vacuo* and forging to $\frac{1}{8}$ -in. diameter bar. The Charpy V-notch impact transition range of this steel, after oil-quenching from 840° C. and tempering at 650° C. followed by water-quenching, was -60° to -200° C. This range was unaffected by exposure for 1,000 hr. at 450° C.

Another steel of the same nominal composition was prepared, using similar raw materials, by melting and casting *in vacuo*. The 22-lb. ingot produced was forged and rolled to $\frac{1}{8}$ -in. diameter bar. After oil-quenching from 840° C. and tempering at 650° C. and water-quenching, the impact transition range was again -60° to -200° C., and the range was unaffected by exposure for 1,000 hr. at 450° C. and water-quenching.

Now it is known that steels can be made, with impact properties which are unaffected by exposure at 450° C., it should be possible to assess the effects of each of the trace elements normally present in commercial materials by studying high-purity steels to which these trace elements have been added in controlled amounts.

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Extension of Field of Application of Relaxation Methods of Computation

THE availability of suitable computing machines makes it possible to consider the solution of sets of non-linear partial differential equations by the progressive reduction of residual errors over networks of points. The example below makes clear the process envisaged. I am not aware of any previous discussion of this process in such a general context.

The theory of turbulent gas jets¹ provides a simple example in which the field equations can be written as follows:

$$U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial r} + \frac{C^2 x^2}{r} \frac{\partial}{\partial r} \left\{ r \left(\frac{\partial U}{\partial r} \right)^2 \right\} = 0 \quad (1)$$

$$\frac{\partial U}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} \{ r V \} = 0 \quad (2)$$

In this case there are two dependent variables U , V ; two independent variables x , r ; and a constant C . The first step is to divide the region of interest into a network of points and take values of U and V at these points. The next step is to calculate the left-hand sides of the two equations at the points of the network and consider these residuals. Adjustments ΔU and ΔV must now be made to the initial values U_0 and V_0 to reduce the residuals to zero. To facilitate this work, $U_0 + \Delta U$ and $V_0 + \Delta V$ are substituted in the equations and only linear terms in ΔU , ΔV retained. Thus equations 1 and 2 become:

$$\begin{aligned} U_0 \frac{\partial U_0}{\partial x} + V_0 \frac{\partial U_0}{\partial r} + \frac{C^2 x^2}{r} \frac{\partial}{\partial r} \left\{ r \left(\frac{\partial U_0}{\partial r} \right)^2 \right\} + \Delta V \frac{\partial U_0}{\partial r} \\ + \Delta U \frac{\partial U_0}{\partial x} + U_0 \frac{\partial \Delta U}{\partial x} + \left\{ V_0 + \frac{2C^2 x^2}{r} \frac{\partial}{\partial r} \left(r \frac{\partial U_0}{\partial r} \right) \right\} \frac{\partial \Delta U}{\partial r} \\ + 2C^2 x^2 \frac{\partial U_0}{\partial r} \frac{\partial^2 \Delta U}{\partial r^2} = 0 \end{aligned} \quad (3)$$