Acta Cryst. (1963). **16**, 839

The Heusler structure of Au_2MnAl.

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(*Received* 21 *December* 1962)

The Heusler structure is body-centred cubic with a face-centred superlattice, and may be thought of as four interpenetrating face-centred cubic lattices A, B, C, and D, of which A and C are identical. In the well-known ferromagnetic Heusler alloys Cu_2MnX, Cu atoms lie on lattices A and C, Mn atoms on B, and X atoms (which may be Al, In, or Sn) on D. The structure factor formula (Bradley & Rogers, 1934) takes the following forms: (1) main lines, $Q^2(=h^2+k^2+l^2) = 8, 16, 24, \ldots$, $F = f_A+f_B+f_C+f_D$; (2) even superlattice lines, $Q^2=4, 12, 20, \ldots$, $F=(f_A+f_C)-(f_B+f_D)$; (3) odd superlattice lines, $Q^2 = 3, 11, 19, \ldots$, $F = \{(f_A-f_C)^2+(f_B-f_D)^2\}^{\frac{1}{2}}$; where $f_A, f_B, \ldots$ are the scattering factors of the atoms on the $A, B, \ldots$ lattices. The structure is distinguishable from the $B2$ or CsCl type, in which lattices B and D are also identical, by reflexions of type (3) if there is a sufficiently large difference in the scattering factors of the atoms on B and D.

In an earlier attempt to discover gold-based Heusler alloys (Morris, Preston & Williams, 1959) this difference proved too small to allow these reflexions to be detected with certainty by conventional X-ray film and microphotometer techniques, although the ferromagnetism exhibited by the alloy at low temperatures suggested that the Heusler structure existed. This has now been confirmed both by neutron diffraction (Bacon, 1962*a*) for which the scattering factors are more suitable, and by our own re-examination with an X-ray diffractometer.

Powder samples annealed at 700 °C for 24 hours or more we examined after different rates of cooling. After quenching of the samples in iced water no reflexions other than the even superlattice and main lines were definitely detected, but after they had been cooled to room temperature over a period of 6 hours two small peaks appeared which were identified as the 111 and 311 reflexions of a Heusler structure of lattice parameter 6·358 Å. A slower cooling rate (over about 3 days) produced additional lines which were indexed as belonging to a second cubic structure of lattice parameter 5·993 Å. This is presumably the Al_2Au phase (Pearson, 1958), so that the equilibrium structure of Au_2MnAl at lower temperatures is two-phase. The results show that the ordered arrangement of the Mn and Al atoms on the B and D lattices is at least partially destroyed on raising the temperature but the X-ray intensities are too small to make any accurate quantitative measurements on the degree of order. The latter however has a marked effect on the magnetic properties, the saturation intensity (extrapolated to infinite field and absolute zero) increasing from about 24 e.m.u.g^{-1} for a quenched sample to about 55 e.m.u.g^{-1} for a slow-cooled sample. The Curie point of the latter is −53 °C. The detailed magnetic measurements and the thermal expansion of Au_2MnAl and $Au_2Mn_{2-x}Al_x$ $(0<x<1)$ will be reported elsewhere.

A comparison of the crystal structures and magnetic properties of AuMn and Au_2MnAl is also of interest. AuMn has a CsCl type of structure and is antiferromagnetic, but the observed magnetic structure (Bacon, 1962*b*) is not that in which nearest neighbours in the simple cubic lattice of Mn atoms are antiferromagnetically aligned. Instead there appears to be a strong antiferromagnetic exchange interaction between the pairs of Mn atoms situated at the ends of a body diagonal. In the Heusler structure of Au_2MnAl every alternate Mn atom along cube edges in AuMn is replaced by Al, so that along ⟨111⟩ directions the sequence of atoms is changed from Mn–Au–Mn–Au–Mn to Mn–Au–Al–Au–Mn. We suggest that the antiferromagnetic coupling in AuMn is due to indirect exchange interaction between Mn atoms via an intervening Au atom. This has been removed in Au_2MnAl and the alloy is ferromagnetic.

We wish to thank the Department of Scientific and Industrial Research for a maintenance grant to two of us (C. D. P. and J. L. H.) and the Council of the Royal Society for a grant-in-aid.

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Acta Cryst. (1963). **16**, 839

Fourth-order elastic coefficients in crystals.

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(*Received* 7 *March* 1963)

Starting from Murnaghan's theory (1937) of finite strain, Birch (1947) considered the theory of finite elastic strain for a medium of cubic symmetry in which the expression for free energy contains third-order strain components. Introducing the concept of effective elastic constants, Chelam (1961) has recently studied the effect of large stresses on elastic solids, and the results he obtained by taking the second-order and third-order strain components in the strain-energy expression are not in complete agreement with the experimental results. To obtain