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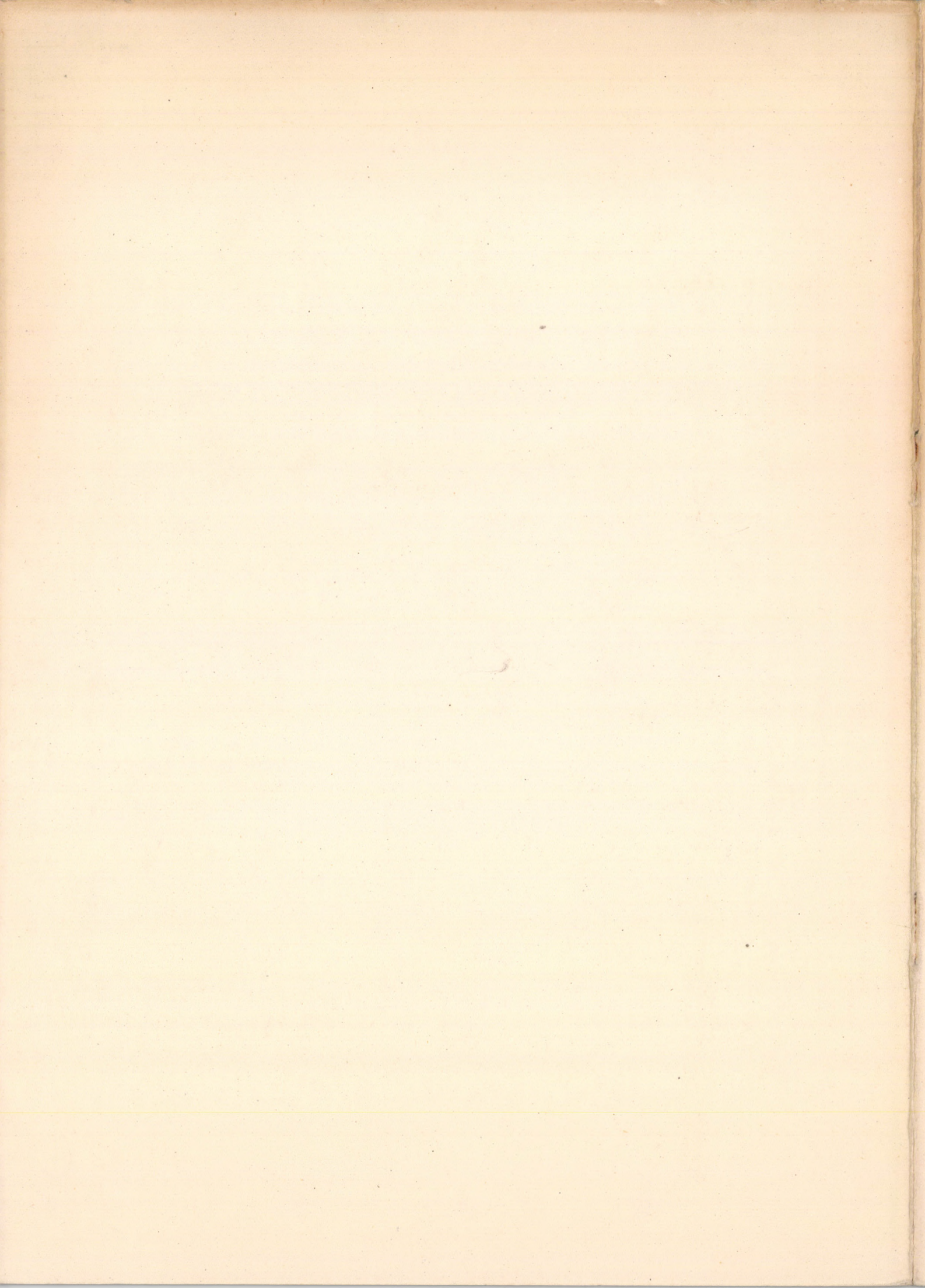
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## ATOMIC AND MAGNETIC ORDER IN $Mn_2Pd_3$

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Abstract. The existence of ordered Pd atoms within the Mn sublattice has been established in antiferromagnetic  $Mn_2Pd_3$  of CuAuI type and its effect on the Néel temperature has been investigated.

Manganese forms with Ni, Pd, Rh, Ir and Pt intermetallic compounds of ordered CuAuI type which are stable in wide ranges of concentration and temperature [1]. They are all antiferromagnetic having the same basic magnetic structure, as determined by neutron diffraction in MnNi [2], MnPt [3], MnPd [4] and  $Mn_2Pd_3$  [5]. In the non-stoichiometric alloys the atoms of the excess component are, generally, distributed randomly on the sublattice of the other. On annealing at  $450^\circ C$ , an unspecified secondary order was, however, observed by X-ray diffraction in the Mn-Pd system near  $Mn_2Pd_3$  composition [6]. Owing to this ordering, first, the temperature associated with maximum susceptibility shifts to higher or lower values, depending on the Mn concentration being less or more than 38 atomic%, second, the susceptibility increases by an order of magnitude and becomes dependent on the field strength [6,7].

In order to establish the crystal and magnetic structures in  $Mn_2Pd_3$  annealed at  $450^\circ C$ , magnetic susceptibility and neutron diffraction measurements were performed. The sample was prepared from 99,9 % purity metals by melting in argon atmosphere. The ingot was filed, then annealed at  $450^\circ C$  for 10 days. The Mn concentration was 40,1 atomic% according to chemical analysis.

At room temperature the neutron diffraction pattern shows reflections characteristic of CuAuI type atomic and MnNi type magnetic order. In addition, some weak superreflections also occur which can be indexed in a

doubled unit cell. These superreflections are assumed to be nuclear, since the form factor would cause a larger decrease for magnetic reflections at high angles. This is an indication of some order in the excess Pd atoms within the Mn sublattice. The unit cell of CuAuI type and the projection of the cell, doubled in three directions, on the (001) plane are shown in Fig.1. The Mn sites are numbered by 1-8 and 9-16 in the planes corresponding to  $z=0$  and 1, respectively. The measurements are compatible with the excess Pd atoms preferring either sites 1, 5, 10, 16 or 1, 5, 12, 16. To decide between the two models, the detection of additional weaker reflections would be required, possibly on single crystal. Either model is associated with  $Mn_3Pd_5$  /37,5 atomic% Mn/ composition.

The temperature dependence of the (100) magnetic peak intensity yields  $T_{N,1}=370\pm 10^\circ$  C/curve A, Fig. 2/. Annealed at  $600^\circ$  C for some minutes, the additional reflections vanish and  $T_N$  shifts to  $340\pm 10^\circ$  C/curve B/. During the measurement the nuclear reflection (001) was constant indicating an unchanged primary CuAuI order /curve C/. For reannealing at  $450^\circ$  C the additional reflections reappear. The magnetic structure, which is the same as in MnPd [4] with  $u_{Mn}=4,3\pm 0,3, u_B$  at  $20^\circ$  C, is not affected by the ordering of the Pd atoms.

The susceptibility results of Fig. 2 are in agreement with those of [6,7]. If the secondary order exists /curve 1/, the susceptibility is higher and the temperature of its maximum is lower than the values without this order /curve 2/. It is seen that the temperature associated with the maximum in curve 2 corresponds to  $T_{N,2}$  determined from curve B. The maximum in curve 1, however, does not represent the  $T_{N,1}$  of the ordered phase. The value of  $T_{N,2}$  is in agreement with [6,7] but, perhaps due to a difference in composition, lower than that of [5]. The shift of  $T_N$  during the secondary ordering may be attributed to a change in the lattice parameters. It cannot be established from present measurements whether the increase in susceptibility is inherent to the secondary ordering.

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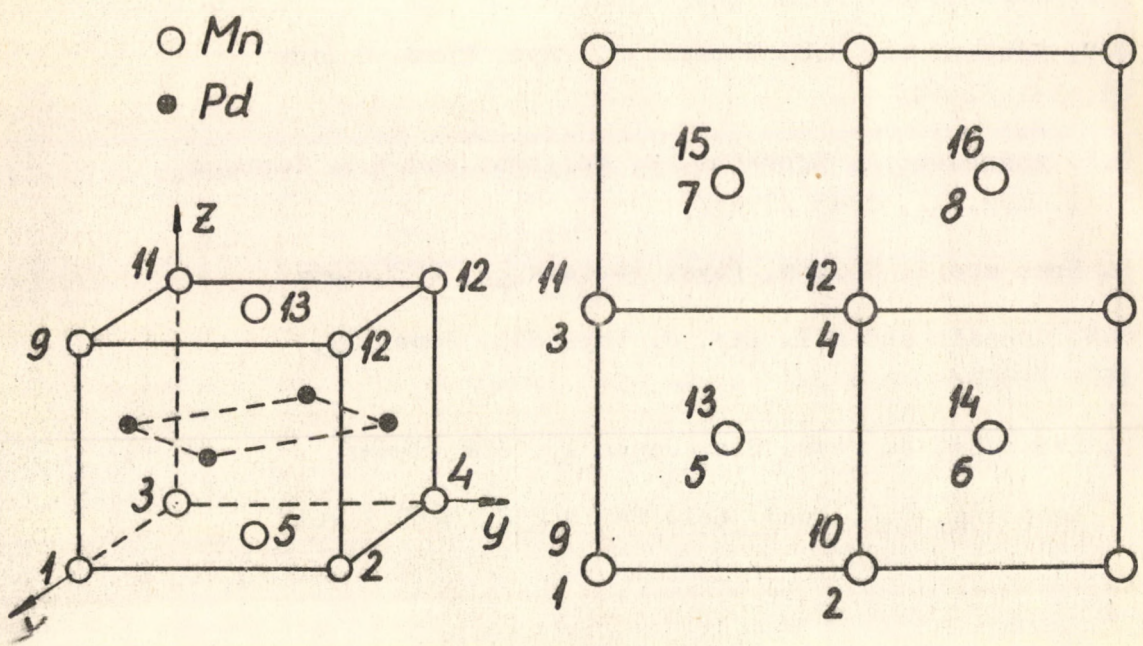


Fig. 1

Unit cell of CuAuI type and projection of the eightfold cell on the (001) plane

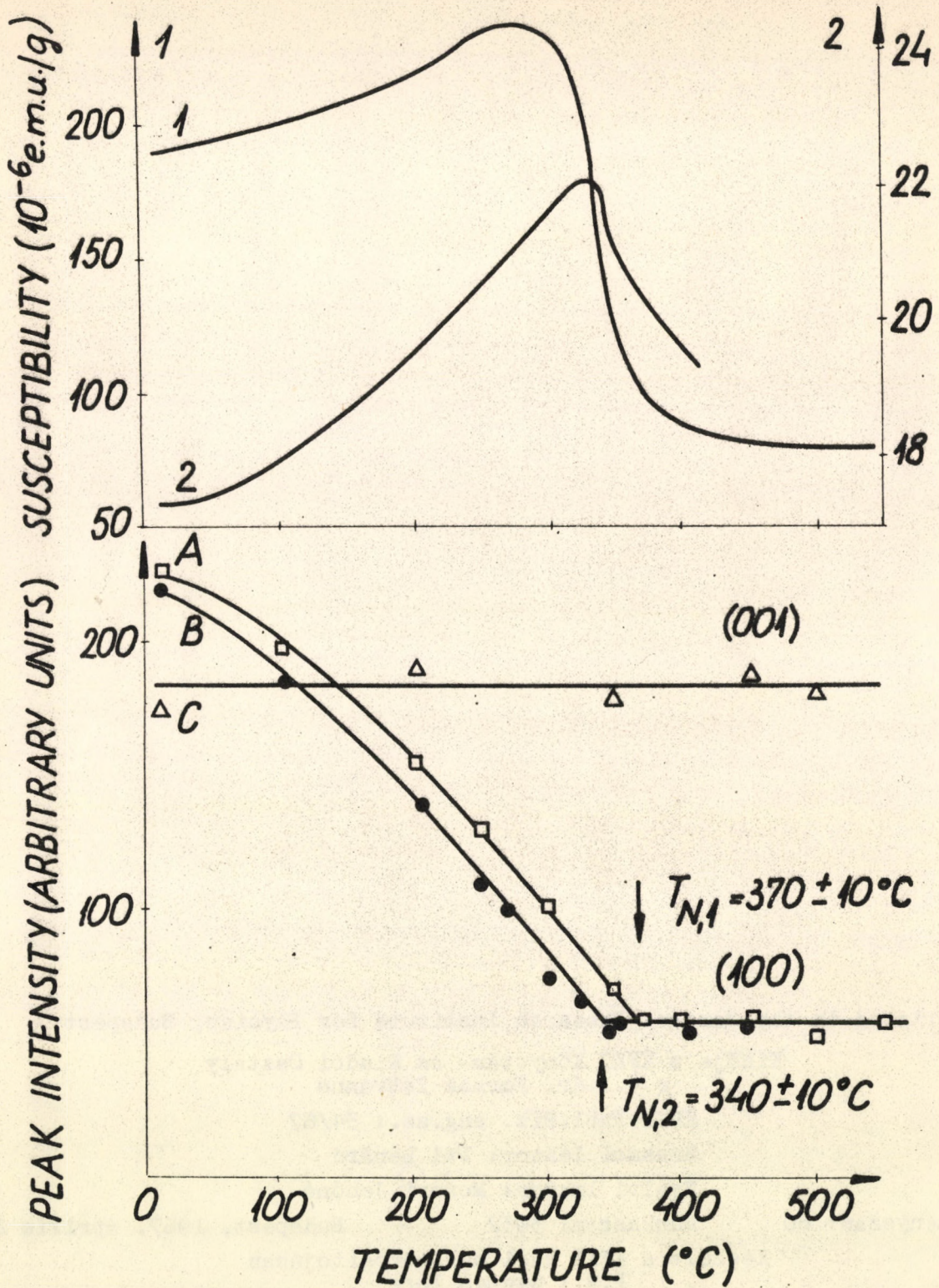


Fig. 2.

Variation of magnetic susceptibility and neutron peak intensities with temperature. Curves A and 1 are taken in the presence, curves B and 2 in the absence of secondary order

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