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X-ray Diffraction Studies of Wüstite at High Temperature*

BY M. HAYAKAWA AND J. B. COHEN

Materials Science Department, The Technological Institute, Northwestern University, Evanston, Illinois 60201, U.S.A.

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Diffuse scattering from Fe_rO was measured at 840°C. Relatively sharp peaks were observed along the [h00] direction near the NaCl-type fundamental peaks. The separation between these peaks and the fundamental peak corresponded to a periodicity of 2.6 times that of the NaCI-type structure in agreement with the measurement on a quenched specimen [Koch, F. & Cohen, J. B. (1969). Acta Cryst. B25, 275-287]. The peaks decreased in intensity smoothly as the composition approached the iron-rich phase boundary. However, even at the closest point to stoichiometry (x = 0.956) the peaks were still intense. Both the peak position and the half breadth of the peak were approximately constant with variation of the composition. For x = 0.900 and x = 0.956, SRO intensity was separated from the total diffuse scattering along the [h00], [hh0] and [hhh] directions. The SRO intensity consisted of the aforementioned peaks and the diffuse portion with a smooth modulation. Fourier transformation of the SRO intensity yielded positive SRO parameters for the first few shells of the octahedral cation sublattice, indicating a clustering trend within the superstructure cell (whose size was known to be on the average 2.6 times of the NaCl-type cell). A computer-simulated structure [Gehlen, P. C. & Cohen, J. B. (1965). Phys. Rev. 139, A 844–A 855] which was forced to fulfil the first six measured SRO parameters shows that the cation vacancies are mostly linked together with $\frac{1}{2}\langle 110 \rangle$ vectors for both compositions. However no particular shape of the vacancy clusters was noticed in the simulation.

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On the Evolution of States from a Non-Equilibrium Solid Solution

By J. W. CAHN

Department of Metallurgy and Materials Science, Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.

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Despite the enormous variety of structural states that evolve from non-equilibrium solid solutions and despite the even larger number of models that have been proposed for them, it is becoming apparent that only a limited number of basic types of evolutionary paths exist. These are determined by considerations of thermodynamic and elastic stability, diffusion mechanisms and interface effects. For many cases, an unambiguous and detailed prediction of structural states is possible that is entirely consistent with both diffraction and imaging experiments. For other cases, strong inferences can be drawn from a few observations that drastically and verifiably limit the range of speculation. When the structure is deduced from these considerations, there are none of the special ambiguities that necessarily resulted when structural states were deduced entirely from diffraction evidence.