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X-ray scattering by lattice defects in neutron-irradiated single crystals of boron carbide. By CHARLES W. TUCKER, JR. and PETER SENIO, Knolls Atomic Power Laboratory*, General Electric Company, Schenectady, N.Y., U.S.A.

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In a radiation-damaged material the lattice defects are usually considered to be isolated interstitial lattice atoms, vacancies, and perhaps rather small agglomerates of these defects. If a sufficiently large concentration of these defects can be built up, it seems reasonable that observable X-ray effects might be found. Further, it would seem, the defects being relatively simple in nature, that the X-ray effects might be interpreted without too much difficulty.

There have been a number of theoretical calculations of the X-ray effects to be expected from localized static lattice defects in crystals. Zachariasen (1945) has given a general theory of displacement disorders. Huang (1947) has given a detailed treatment of the X-ray effects to be expected from spherically symmetric elastic singularities in a face-centered cubic lattice. Both of these treatments show that the intensities of the Laue-Bragg maxima are altered, as if by an artificial temperature effect, and that there is no broadening of the Laue-Bragg maxima due to the defects. Huang's analysis also predicts an isotropic expansion of the lattice, which can be shown to lead to Vegard's law for the case of solid solutions. The absence of line broadening in solid solutions provides a further test of the calculations of Zachariasen and of Huang. Both analyses also predict that the defects should produce diffuse maxima surrounding the reciprocal-lattice points.

Boron carbide, B₄C, suggests itself for a study of X-ray scattering by localized static lattice defects because, owing to its high melting point and great strength, it might be expected that the defects once formed would have little tendency to anneal out at ordinary temperatures. Radiation damage in boron carbide is produced mostly by the reaction of the B-10 nucleus with thermal neutrons to form He-4 and Li-7 nuclei, which then dissipate (Bethe, 1950) 1.47 and 0.84 MeV., respectively, of kinetic energy in ionization and bumping collisions. The importance of this reaction is due to the high cross section (4000 barns) and isotopic concentration (15% of all atoms in $B_{4}C$) of the B-10 nucleus. These factors afford an excellent means of producing a large amount of relatively stable damage quickly with very little attendant radioactivity.

We have had single crystals of boron carbide irradiated in thermal neutron fluxes for a very wide range of exposures and have found all of the effects predicted by the theoretical work of Zachariasen (1945) and Huang (1947). The effects become more pronounced with increasing exposure. Since there is no indication that the nature of the effects changes with increasing exposure, the results for crystals given the heaviest exposure (integrated thermal neutron flux of 3×10^{20} neutrons/cm.²) will be described. There are extensive changes in the intensities of Laue-Bragg maxima. The changes are of two types. First, there is a strong and highly anisotropic artificial temperature factor present. The factor is roughly four times as great in the c_0 as in the a_0 direction.[†] Secondly, there are changes in the intensities indicating real structural differences, i.e. alterations in the average positions of the lattice atoms. There are no apparent changes in the breadth of the Laue-Bragg maxima. Finally, there is an expansion of the a_0 axis of about 0.6% and a contraction of the c_0 axis of about 0.8%. The diffuse scattering around the reciprocal lattice points predicted by Zachariasen (1945) and Huang (1947) is also observed to a very extreme degree. In fact, the integrated intensities of some of the diffuse maxima appear to exceed by a large margin the intensities of their corresponding Laue-Bragg maxima.

The interpretation we give these results is that, owing to anisotropic bonding of displaced lattice atoms and preferential removal of certain lattice atoms by the B-10 reaction and by rearrangement after collision events. there are large local anisotropic distortions of the lattice which give rise to the wide variety and very pronounced X-ray scattering effects covered in a general way by the calculations of Zachariasen (1945) and Huang (1947). These effects seem quite clearly to have such an origin rather than being true thermal effects because the observed effects are not altered by lowering the crystal temperature to that of liquid nitrogen. Although defect scattering has been observed before, for example, in diamond by Lonsdale (1942) and in cold worked metals by Guinier (1939), we have hopes of learning something about the detailed nature of the defects in irradiated boron carbide. To accomplish this, we plan to use the theory of Zachariasen (1945) and perhaps also to extend the analysis of Huang (1947) to the case of anisotropic defects. For this work we are currently conducting Fourier analyses of the intensities of the Laue-Bragg maxima and also plan to study the intensities and shapes of the diffuse maxima. The results of these studies will be given in full at a later date.

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[†] The crystal structure of boron carbide has been shown by Zdanov & Sevastianov (1941) and by Clark & Hoard (1943) to be rhombohedral. The a_0 and c_0 refer to the axes of the corresponding hexagonal unit cell.