

DIFFUSION OF He INTO SOLID C₆₀ FROM X-RAY DIFFRACTION DATA.

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In crystalline C₆₀ there are two tetrahedral and one octahedral cavities per fullerite molecule; the mean diameters of which are respectively 2.2 Å and 4.2 Å [1,2]. This allows an easy preparation of fullerite-based interstitial solutions over a wide range of dopant concentrations. For some types of impurities (for instance, alkali metals), there is a more or less generally accepted physical viewpoint concerning the effects brought about by the impurities, for other (for instance, rare gases or simplest linear molecules), such a unified concept is still to be worked out. Addressing, specifically, rare gas species as intercalants, we note that effects of saturation of C₆₀ with helium have been scarcely studied [3, 4]. It is more so surprising that experimenting with helium as intercalant does not call for elevated pressures to reach sufficiently high helium concentrations in C₆₀, though it is quite reasonable to expect that saturation kinetics as well as consequences of intercalation will bear much similarity with results for other small-size intercalant species.

The processes of helium diffusion into polycrystalline C₆₀, intercalated at room temperature and the pressure of about 1 atm., were investigated by x-ray powder diffraction. The intercalation was performed during 4000 hours with periodical X-ray photography. It was determined that intercalation with He atoms leads to essential distortions of the C₆₀ matrix lattice. Analysis of the temporal variations of the lattice parameter as well as the reflection intensities and halfwidths (saturation level) during both intercalation and degassing processes allows us to claim that the voids of the C₆₀ lattice are filled in two stages. At the first stage octahedral cavities are filled up (subsurface layers first, than deeper layers of the crystallites). During the second, longer, stage, diffusive penetration of impurities into the tetrahedral cavities takes place. Macroscopic equations of such a two-stage intercalation are formulated. Comparison of calculated and experimental curves lead us to a few conclusions about the energy parameters that control the He diffusion process.

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4. K. Ichimura, K. Imaeda and H. Inokuchi, *Mol. Cryst. Liq. Cryst.* **340**, 649 (2000).

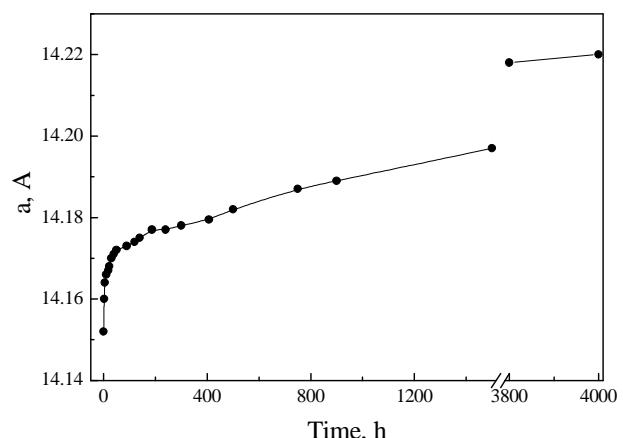


Fig 1. Dependence of the lattice parameters on the intercalation time

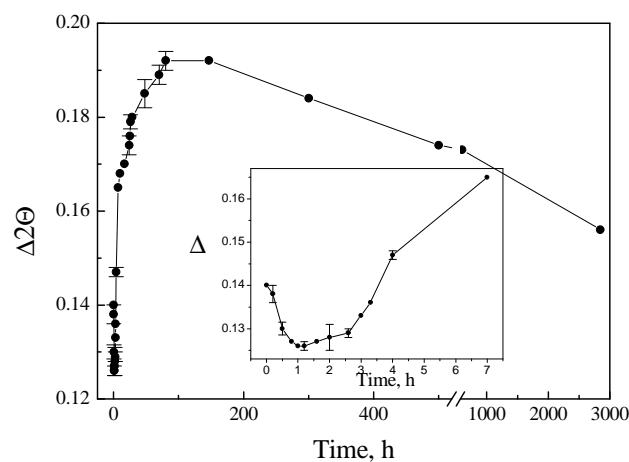


Fig 2. Dependence of the line half-width on the intercalation time

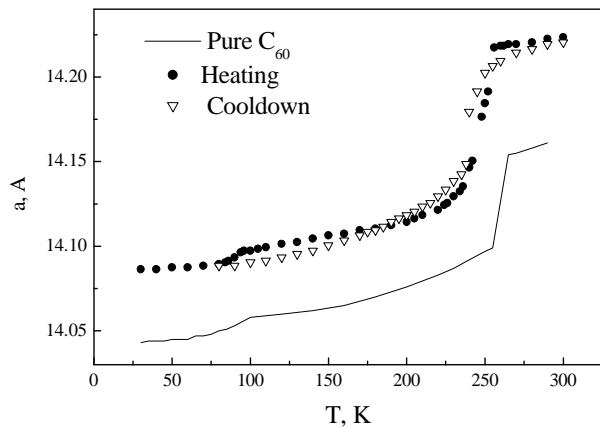


Fig 3. Temperature dependence of the lattice parameters for helium saturated and pure specimens