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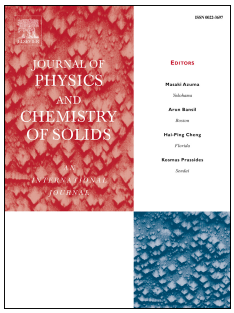

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Effect of high-energy mechanical milling on the FSDP-related XRPD correlations in Se-rich glassy arsenic selenides

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Abstract

The X-ray powder diffraction (XRPD) patterns related to the first sharp diffraction peak (FSDP) are registered for Se-rich As_xSe_{100-x} glasses ($5 \le x \le 40$), subjected to high-energy mechanical milling in a dry mode with 500 min^{-1} rotational speed. The results are treated in terms of structural model assuming broad diffraction halos in the XRPD patterns appeared due to remnants of *inter-planar* "quasi-crystalline" correlations, disturbed by overlapping with diffuse halos originated from strongest *inter-atomic* correlations, in part, the nearest-neighbor correlations between cation-like atoms. Milling does not influence the FSDP in a vicinity of glassy Se ($x<20$), while causes increase in the FSDP width ΔQ (the reduced correlation length L) in the glasses with $20 \le x < 40$, these changes being ascribed to disturbed inter-planar arrangement in covalent-bonded network due to structural defects generated under attrition ball milling. Assuming contribution of the Ehrenfest diffraction from coordination spheres in the detected XRPD patterns, the latter is ascribed to broadening in the distribution of characteristic FSDP-related inter-atomic distances, thus testifying in a favor of more defective structure of milled glass.

Key words: glass; arsenic selenide; mechanical milling; X-ray powder diffraction; first sharp diffraction peak.