Abstract Submitted
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Microscopic Origin of Polarity in Quasi-Amorphous BaTiO3.[1] A.I. FRENKEL, Yeshiva University, New York, Y. FELDMAN, V. LYAHOVITSKAYA, E. WACHTEL, I. LUBOMIRSKY, Weizmann Institute of Science, Israel — The recent observation of pyroelectricity in quasi-amorphous thin films of $BaTiO_3$ introduced a previously unreported type of polar ionic solid where the appearance of a macroscopic dipole moment is not accompanied by long-range crystal-like order. This poses a question regarding the mechanism of polarity in non-crystalline ionic systems and the nature of their local dipoles. By combining X-ray diffraction and X-ray absorption fine structure spectroscopy techniques we have identified the local dipoles as stable but distorted TiO_6 octahedra. The magnitude of the off-center displacement of the Ti ion and the concomitant dipole moment in both quasi-amorphous (polar) and amorphous (non-polar) $BaTiO_3$ were found to be nearly twice as large as those in bulk $BaTiO_3$. We propose that the mechanism of macroscopic polarity in quasi-amorphous $BaTiO_3$ is in a weak orientational ordering of the TiO_6 bonding units. In this view, one may expect that other amorphous ionic oxides containing stable local bonding units, for example NbO_6, TiO_6 or VO_6, may also form non-crystalline polar phases.

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Anatoly I. Frenkel
Yeshiva University

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