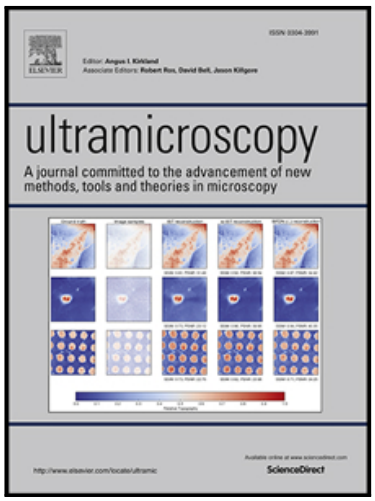

Using Molecular Dynamics for Multislice TEM Simulation of Thermal Diffuse Scattering in AlGaN

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Highlights

- molecular dynamics simulations used to determine thermal displacements
- used for frozen phonon simulations of CTEM and STEM
- Stillinger-Weber type potential derived for the thermal dynamics of AlGaN
- displacement calculations in alloys including correlation
- comparison to quantum mechanical calculated results shows very good agreement