

# Warm Dense Crystallography

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The femtosecond scale of intense x-ray pulses from x-ray free electron lasers (XFELs) is now well established as being able to create interesting states of matter characterized by long-lived non-equilibrium semicore or core electron occupancies or by the heating of dense phases via the relaxation cascade initiated by the photoelectric effect. We address here the latter case of so-called ‘warm dense matter’ (WDM) and seek to better understand how experiments can be best designed to investigate the consequences of electronic heating in tepid WDM states of crystalline phases where the lattice degrees of freedom have insufficient time to respond. We report temperature-dependent density functional theory calculations for the x-ray diffraction from perfectly crystalline LiF, graphite, diamond, and Be. We find strong signatures of condensed-phase effects that are testable by experiment and that emphasize the importance of wide-angle scattering, i.e., that requires the use of high energy x-rays to obtain the Bragg intensities for a wide range of momentum transfers.

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