

STABILITY OF LiF CRYSTAL IN THE WARM DENSE MATTER STATE

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The finite temperature density functional theory approach is deployed for description of the fcc LiF crystal in a two-temperature warm dense matter state with hot electrons and cold lattice that is formed after ultrafast energy deposition. The lattice stability and the interatomic bonding at elevated electronic temperatures are studied. The excitation of the electronic subsystem at temperatures $T_e \sim 3\text{eV}$ results in the loss of mechanical stability of the fcc LiF lattice that is manifested as an appearance of the soft acoustic phonon mode and should probably lead to non-thermal melting. The corresponding redistribution of the electronic density implies that the originally strongly ionic interatomic interaction becomes more of covalent character with the rise of electronic temperature.