Distortions and low Symmetry Environments in Liquids : Alkalis at High Pressure

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The melting curve of sodium measured in exhibits totally unexpected features under pressure : the melting temperature, Tm, reaches a maximum around 30 GPa followed by a sharp decline from 1000 K to 300 K in the pressure range from 30 to 120 GPa.

In the present study, the structural and electronic properties of molten sodium and lithium are studied using first principles theory. With increasing pressure, both liquids evolve by assuming a more compact local structure, which accounts for the maximum of Tm at 30 GPas in Na and the flattening of the melting curve in Li. However, at pressure around 65 GPa in Na and 20 GPa in Li a transition to a lower coordinated structure takes place, driven by the opening of a pseudogap at the Fermi level. Remarkably, the 'broken symmetry' liquid phase emerges at rather elevated temperatures and above the stability region of a closed packed free electron-like metal. The theory explains the measured drop of the sodium melting temperature, down to 300 kelvin at 105 GPas. The behavior of Li at higher pressure is even more surprising as we evidence the emergence of tetrahedrally (slightly) bonded clusters as due to increased core-core overlap.

The properties of the proposed new liquid phases and the implications of our findings for the stability of low-symmetry solids will be discussed.

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