New insights on metals under extreme conditions

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Organisers

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Introduction and motivation

In the recent years, large efforts have been devoted to the description and understanding of the transformations undergone by metals under high pressure and temperature, in particular upon melting. The main difficulty for theoreticians is to handle matter under high temperatures, where atoms no longer follow simple harmonic motion and may even undergo electronic excitations. While theory often predicts well stable phases at low temperatures, it has difficulty with high temperatures. On the experimental side, attaining and measuring pressures of a few millions of atmospheres and temperatures of several thousands of K, and at the same time, reaching and identifying the equilibrium state of the material it is also a great challenge.

A likely result of these difficulties is the remarkable controversy which remains for the effect of pressure on the melting point of several metals. Up to recently, the melting curve $T(P)$ of these metals (Mo, Ta, W, Ni, Fe…) obtained from laser-heated diamondanvil cell experiments was much flatter than those obtained by shockwave experiments, piston-cylinder apparatus measurements and calculations. This discrepancy raised questions on the transformation observed with these different techniques as well as high temperature modelling with DFT. In addition, there was an almost complete lack of structural information on the solid and liquid phases of elemental metals under extreme conditions: even if iron is the focus of numerous studies, its stable phase under the conditions of the Earth's core is still debated.

State-of-the-art

On the theoretical side, quantum molecular dynamics simulations are widely used to predict melting curves or liquid properties under pressure, although their appropriateness may be questioned (size effects…).
Recently, new melting diagnostic have been used, new insights on the structure of liquids have been obtained.
We want to give the specialists (both theoreticians and experimentalists) of all the techniques involved in melting and high pressure-high temperature studies the opportunity to confront their observations and predictions and discuss critical points.

Among those points:

- simulation tools : e.g. quantum molecular dynamics, classical MD, LOTF techniques
- equations of state and anharmonicity in solid phases
- models for liquid metals
- static vs dynamic melting
- metrology: pressure and temperature measurements
- metastability
- thermal transport
- chemical reactions in DACs
- shock pyrometry
- etc.

Future developments will be discussed:

- melting diagnostics
- time-resolved techniques

Objectives

The aim of this discussion meeting is to prepare a full scale CECAM workshop, to be held within mid 2012, together with two other co-organizers.

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