

Abstract Submitted  
for the SHOCK11 Meeting of  
The American Physical Society

**Theoretical phase diagram of beryllium at low pressure and high temperature** GREGORY ROBERT, PHILIPPE LEGRAND, STEPHANE BERNARD, CEA DAM/DIF — Beryllium, although a “simple” metal remains a challenge for both theory and experiment. In this presentation, we will try to shed some light on a controversial issue concerning the phase diagram at low pressure and high temperature which is not clearly established [1,2]. In a previous work, we have shown that the bcc structure could be stabilized at high temperature by anharmonic effects [3] and could lead to a bcc pocket located at low pressure-high temperature. This is consistent with recent heated DAC experiments [4]. However to determine if the bcc phase has the lowest Gibbs free energy compared to hcp, we apply the force matching method fitted on quantum molecular dynamics data.

[1] M. Francois and M. Contre in Proc. Grenoble 1965, PUF Paris (1966).

[2] A. Abey in UCRL53567 (1984).

[3] G. Robert et al Phys Rev B 82, 104118 (2010).

[4] Evans et al. cited in Phys. Rev. B 79, 064106 (2009).

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Date submitted: 08 Feb 2011

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