Iron under extreme conditions

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I will report the latest theoretical data on the iron phase diagram. A particular emphasis will be on the stabilization of the high-PT body-centered cubic (bcc) Fe under conditions of the Earth Inner Core[1] and how its stabilization interfere in the interpretation of iron melting curve and resolution of related enigmatic questions.

The mechanism of the high-PT bcc Fe phase stabilization is quite unique. The atoms in this structure move at times as in a liquid[2]. Therefore, the mean square displacement never saturates and the diffusion coefficient and the viscosity of the bcc Fe are similar to those in very viscous liquid[3].

Recently, our theoretical prediction of the stability of high-PT bcc Fe phase[1,4] was confirmed by diamond anvil cell experiments[5]. Interesting, that when a number of the experimental studies analyzed with the knowledge of the physics of the bcc Fe phase, those experiments confirm the stability of the new phase rather than contradict it.

I will show how the X-ray diffraction pattern of the bcc Fe looks like and discuss whether similar XRD patterns have already been observed in Fe high-PT melting experiments. I will demonstrate that the stabilization of the bcc phase was at times misinterpreted as melting.

The similarity of the bcc and liquid iron under extreme conditions of pressure and temperature revives the speculations on the existence of the critical solid-liquid point.

[1] A. B. Belonoshko, T. Lukinov, J. Fu, J. Zhao, S. Davis, S. I. Simak Nature Geoscience **10**, 312 (2017).
[2] https://www.youtube.com/watch?v=s5Rl7mtxiEY
[3] A. B. Belonoshko, J. Fu, T. Bryk, S. I. Simak, M. Matessini, Nature Communications **10**, 1-7 (2019).
[4] A. B. Belonoshko, R. Ahuja, B. Johansson, Nature **424**, 1032 (2003).
[5] R. Hrubiak, Y. Meng, G. Shen, arXiv:1804.05109 Experimental evidence of a body centered cubic iron at the Earth's core conditions.