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Report:

Silicon single crystals used for ultra-large-scaled integrated circuit (ULSI) devices are grown from molten silicon by using the Czochralski (CZ) method. In order to obtain high-quality silicon crystals without defects, understanding of the microscopic crystal-growth processes is very important.

To this goal, the atomic structure has been studied, but the understanding is not complete yet. Molten silicon structure can be determined through x-ray diffraction or EXAFS study. However, an experimental approach to this problem is usually difficult; only two experiments have been carried out using x-ray diffraction [1,2]. In this context, to make the detailed structures of molten silicon in a wide temperature range clear, we focus on the temperature dependence of the structure factor S(Q) of molten silicon, particulary the shoulder of the first peak in the structure factor S(Q) in the deeply undercooled region.

Diffraction measurements were made at ID9. Diffraction signals were detected by an energy-dispersive method at eleven temperature points in a wide temperature range from 1130 to 1620°C including undercooled region of 290°C, using a liquid-nitrogen-cooled Ge solid-state detector. The scattering angle was varied from 2 to 15 degrees in order to obtain S(Q) in a wide Q-scale. Undercooling was achieved through electromagnetic levitation, avoiding heterogeneous nucleation induced by container walls. The levitation chamber was filled with helium gas, which was used for temperature stabilization. Because solid silicon is not metallic, we used a carbon susceptor for pre-heating in order to melt and levitate sample [3]. Pure silicon single crystal spheres ~10 mm in diameter were levitated and melted. Temperature was monitored by a pyrometer, and a video system was used to monitor the sample. The temperature was calibrated at the freezing point of liquid silicon by solidifying and melting the sample.

Figure 1 shows the structure factor S(Q) of molten silicon extracted from measured x-ray scattering intensity data at eleven temperatures. The structure factor of molten silicon has a first peak with a shoulder on the high-Q side. It was confirmed that there is no anomalous behavior around the melting point of bulk silicon.

[1] S. Ansell, S. Krishnan, J. F. Felten and D. Price, J. Phys. C10 (1998) L73.

[2] Y. Waseda, K. Shinoda, K. Sugiyama, S. Takeda, K. Terashima and J. M. Toguri, Jpn. J. Appl. Phys. 34 (1995) 4124.

[3] M. Langen, T. Hibiya, M. Eguchi and I. Egry, J. Crystal Growth 186 (1998) 550.

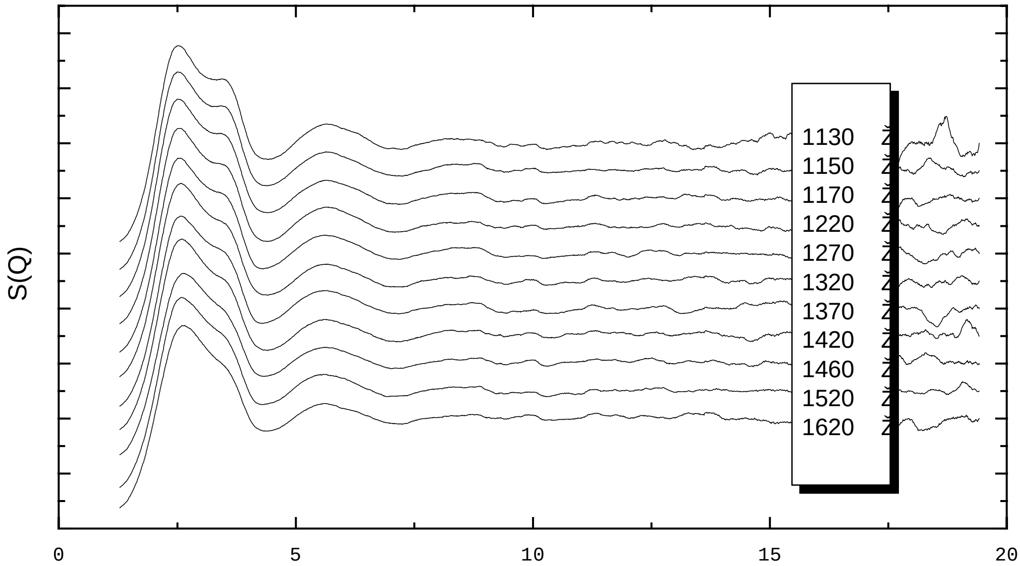

Fig.1 Structure factors of molten silicon at eleven temperatures around melting point