NOVEL PROCEDURE FOR DETERMINATION OF THE MELTING TEMPERATURE OF SPHERICAL NANOPARTICLES IN DILUTE SOLUTIONS AS A FUNCTION OF THEIR RADIUS BY EXCLUSIVELY USING THE SAXS TECHNIQUE

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The purpose of this investigation is to determine the melting temperature of dilute sets of spherical nanocrystals as a function of their radius, by using a novel procedure exclusively based on SAXS results. This procedure relies on the sensitivity of the SAXS function to small and rather sharp variations in size and electron density of nanocrystals at their melting temperature. This method is particularly useful for studying diluted solutions of spherical nanocrystals with wide radius distributions. Other procedures using combined SAXS and WAXS measurements [1] and only SAXS results but in this case referring to systems with narrow size distribution [2] were previously developed.

The input in this procedure is a set of experimental SAXS intensity functions for varying temperatures. In practice, the sample is heated from a minimum temperature lower than the melting temperature of the smallest nanocrystals up to a temperature higher than the melting temperature of the largest nanocrystals. The SAXS intensity is recorded in situ at different temperatures along the whole heating process. The proposed novel procedure was applied to several samples composed of dilute sets of spherical Bi nanocrystals with wide radius distributions embedded in a sodium-borate glass.

Several theoretical models were used for describing the radius dependence of the melting temperature of spherical nanoparticles. One of the most successful analytical model was proposed by Shi [3][4]. In this model, the melting temperature is determined in terms of Mott's theory that accounts for the vibrational component of the melting entropy.

The temperature versus radius function was determined for Bi nanocrystals using the proposed method. Our results agree well with those reported in previous experimental studies using other methods. They also evidence the predicted size-dependent contraction of Bi nanocrystals induced by differences in surface-to-volume ratio of small nanocrystals [5]. An additional size-independent compressive stress - caused by the solid glass matrix in which liquid Bi nanodroplets are initially formed - was also evidenced. This last effect is a consequence of increase in volume of Bi nanoparticles upon crystallization and differences in the thermal expansion coefficients of the crystalline phase of Bi and glass matrix. The additional stress leads to a decrease of about 10 K in the melting temperature of Bi nanocrystals confined in the glass matrix. The procedure described here also allowed us to determine the specific masses and thermal expansion coefficients of Bi nanoparticles in both, liquid and crystalline, phases.

Palabras clave: SAXS, nanocrystals, melting temperature.

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