SIZE DEPENDENCE OF MOLYBDENUM MELTING AND CRYSTALLIZATION TEMPERATURES

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Based on the RP-model, presented in [1], the state equation (P) of molybdenum has been calculated. Interatomic interaction was described by the Mi-Lennard-Jones pair potential. The potential parameters were determined by fitting to the state equation, the bulk modulus, and the coefficient of thermal expansion of molybdenum [2].

Proceeding from the Lindemann criterion under isobaric conditions ($P = 0$), the melting temperature (T_m) has been calculated for nanocrystals with different size and surface shape. It was found that the value T_m decreases with the decrease of the atoms number (N) in the nanocrystal, and it is more noticeable when the shape deviates from the most energetically optimal (a cube for the RP-model).

The surface pressure compress the nanocrystal and to keep isobaric conditions $P = 0$ the interatomic distance must be increased that facilitates melting process.

For the RP-model curves $T_m(N, P = 0)$ end at N_{cr} – minimum possible size of a nanocrystal. For a cube $N_{cr} = 10$, and N_{cr} increases with the nanocrystal shape deformation. If we assume that the value of N_{cr} is the size of the crystalline nucleus with the particular surface shape at $P(N_{cr}) = 0$, then we can get the size dependence of the crystallization start temperature T_{cr}. Extrapolation of the isobaric dependence $T^*_{cr}(N_{cr}^{-\frac{1}{3}}) = T_{cr}(N_{cr}^{-\frac{1}{3}})/T_m(\infty)$ to a macrocrystal ($N_{cr}^{-\frac{1}{3}} = 0$) showed that the value $T^*_{cr}(N_{cr}^{-\frac{1}{3}} = 0)$ is 0.713 for rod-like and 0.857 for plate-like shapes of the nanocrystal. This agrees with the Tarnbull rule, which allows us to state that obtained dependence $T^*_{cr}(N_{cr}^{-\frac{1}{3}})$ describes the dimensional dependence of the molybdenum crystallization start temperature at $P = 0$.

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