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On the disadvantages of the article „Study of primary nanocracks of atomically smooth metals“ (V.M. Yurov, V.I. Goncharenko, V.S. Oleshko)

© M.N. Magomedov

Institute for geothermal problems and renewable energy — branch of the joint Institute of high temperatures of the Russian Academy of Sciences, Makhachkala, Russia
E-mail: mahmag4@mail.ru

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It has been pointed out the groundlessness and inconsistency of the authors' statements in the article [1], as well as the physical and mathematical errors they made.

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A „new analytical model for calculating the characteristics of primary cracks that appear in atomically smooth metals“ has been proposed recently in [1]. However, several issues with the justifiability of claims made in [1] and the results obtained therein presented themselves in the course of reading of this paper. Let us examine these issues in more detail.

The authors of [1] separate a crystal into two phases: phase γ_1 is the surface layer with thickness R_1 and γ_2 is the „bulk phase.“ It is stated that „since surface energy γ_1 of the γ_1 phase layer is three times lower than surface energy γ_2 of the bulk phase, the origin of fracture of metals is at the surface layer“. However, it is known that the notion of surface energy is applicable to the surface only and the authors of [1] do not explain how surface energy γ_2 is determined for the bulk phase. It is also unclear on which grounds do the authors postulate that $\gamma_2/\gamma_1 = 3$ for crystals of all substances at arbitrary temperature. No reference to the source of this statement and no considerations proving it to be true are provided in [1]. Moreover, it is explained below formula (3) that the surface energy at the interphase boundary (γ_{12}) „is negligible in virtue of a second-order phase transition.“ However, from what considerations it was concluded that there is a phase transition of the second kind between the surface and the volume, it is not explained in [1].

The following new concepts are also introduced in [1]. In the opening paragraph of the paper, the concept of a „primary crack“ with its length L „equal to thickness R_1 of the surface metal layer“ is introduced. Several reasonable questions then arise: what is a „primary crack“ and does a „secondary“ one exist? No answers to those questions are provided in [1]. Having postulated that $L = R_1$, the authors of [1] then pose a question: „What are the sizes of primary nanocracks of atomically smooth metals?“ However, the terms „nanocrack“ and „primary nanocrack“ remain undefined. With that, the authors state that the aim of the study „is to develop a calculation procedure, calculate

the length of nanocracks... and compare the results with the Griffith theory.“ However, since $L = R_1$ has already been postulated in (1), what is the point to „develop a calculation procedure“ for the nanocrack length? A crack is a discontinuity of a solid, but how a crack is defined at the nanolevel? This was not done in [1].

Function σ_{is} is introduced in formula (4) as „internal stresses between phases γ_1 and γ_2 .“ It follows from the summary table that the value of σ_{is} in metals is on the order of tens of GPa (1 GPa = 10 kbar = 10 000 atm). However, the authors do not explain why phases γ_1 and γ_2 do not separate under such stresses. It is also unclear why equilibrium thermodynamics formulae should remain applicable under such pressure gradients.

As is stated in [1] below formula (8), „It was demonstrated in our study that a primary nanocrack develops due to noncompensation with atoms located on the surface and in the bulk.“ A question then arises: what „noncompensation with atoms located on the surface and in the bulk“ is being referred to?

The use of formulae in [1] also raises many unresolved questions. The measurement units in formulae (1) and (2) do not match. Note that formula (2) was derived from an empirical plot presented in [2]. However, study [2] is not cited in [1]. Moreover, it is claimed that formula (2) was obtained by Yurov et al. in [3]. It is also stated that (2) contains „surface energy of bulk metal γ_2 .“ However, formula (2) was derived in [2] not for a solid „bulk“ phase (as is claimed in [1]), but for simple surface tension of a liquid phase.

Formula (8) does not follow from (7), since both terms in (7) are positive and L_G is in the numerator. The strangest thing of all is that the following relation is easy to obtain by inserting (4) and (3) into the left- and right-hand parts of Eq. (8):

$$L_G = (2/\pi)R_1 = 0.6366R_1. \quad (A)$$

It then becomes clear why $L_G < R_1$ in the table in [1]. Notably, result (A) and the results in the table differ

significantly from equality (1) postulated by the authors (i.e., $L = R_1$).

The statements (found below Eq. (8)) that „this model is applicable not just to metals; it holds true for any solids, polymers and minerals included“ and that „the proposed model is universal in nature“ become understandable in light of result (A). A question then arises: why only the „atomically smooth metals“ are featured in the title of [1]?

In the concluding paragraph of [1], the authors state that „calculated Griffith length L_G of a crack differs from crack length L by 9% on the average, thus providing support for our theory.“ However, this consistency with the „Griffith crack model“ does not bode well for the authors of [1]. The thing is that Griffith considered a crack in the bulk of a material [4] and his criterion turned out to be not entirely correct in quantitative terms. In addition, the Griffith criterion yields an infinite strength at zero crack length (i.e., in transition to nanocracks). This has been pointed out by Frenkel as early as in 1952 [5], and more current data on calculations of the critical crack length may be found in [6]. Therefore, it was reasonable for the authors of [1] to rely on more modern research [5,6] instead of the Griffith criterion. In addition, once the authors [1] decided to examine cracks at the nanolevel, they should have taken into account the fact that all metals parameters which used in [1] (density, surface energy, melting point, Young’s modulus, etc.) become dependent at this level on the size of the system within which they are applied [7].

It is stated in the abstract of [1] that „for the first time, the parameters of primary cracks were calculated using the example of atomically smooth metals.“ However, a contradictory statement is made later on: „It is shown that our results are consistent with previously known results.“ Where is then the novelty of this study?

Thus, many groundless allegations are found in [1], and the reported results are incorrect and do not characterize the process of crack formation in metals or other solids.

Conflict of interest

The author declares that he has no conflict of interest.

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