Discussion

Discussion of “A Molecular Dynamics Simulation Study of the Cavitation Pressure in Liquid Al”*

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The recent report by Hoyt and Potter using molecular dynamics to simulate cavitation in liquid aluminum selects an unusually low value for the interatomic potential, which leads to an unusually low value for the tensile strength of liquid Al. A revised value for the interatomic potential results in a cavitation pressure consistent with other estimates of this parameter.

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The interesting and welcome report by Hoyt and Potter^[1] on a molecular dynamics (MD) estimate of the fracture pressure of liquid Al contains much of interest, including the significant findings that solute atoms (Mg in this case) and solidification fronts are not the preferred initiation sites for cavitation.

A concern with this excellent piece of study lies with the selection of the interatomic potential. This seems worryingly low. The authors draw attention to the fact that it is consistent with a surface tension $\gamma = 280$ mN/m. Using this value, the cavitation pressure from their study is found to be close to 1340 MPa. This is very much smaller than other estimates for this parameter (the further interesting correction for volume and time used by the authors to reduce this value by a further factor of 2 is neglected for the moment to make comparisons with other researchers, who in general have overlooked this correction).

For instance, a reasonable estimate of fracture pressure of a liquid metal can be deduced from the

elementary equation for the mechanical stability of a bubble: $\Delta P = 2\gamma/r$. Assuming a value for surface tension as determined by nearly all the most recent reliable techniques, which report values approximately four times higher than that implied in the authors' study, close to 1000 mN/m, and assuming a bubble radius of one atom diameter 0.286 nm^[2] (to give an embryonic bubble consisting of approximately 8 vacancies), the fracture pressure is estimated to be close to 7 GPa. Increasing the fracture pressure of the authors by a factor of 4 gives a value of about 5.4 GPa which holds as good an agreement as might be expected. These higher values are corroborated by other authors using MD calculations. For instance, studies by Milstein *et al.*^[3] indicate that a tensile stress of over 15 GPa (with a surface tension approaching 2000 mN/m) is required to stabilize a void in Ni, causing it to grow explosively to promote failure.

The preoccupation of the authors with the inability to correlate with hot tearing stresses is easily explained. Nearly all liquid metals, and in particular Al alloys, are filled with a dense population of macroscopic unbonded interfaces which I have called bifilms. These interfaces occur naturally during the stirring and pouring of liquid metals. The fracture pressures can consequently reduce to nearly zero depending on the size of these entrained defects. The extensive evidence for their existence and their important effects on properties is summarized in a recent book.^[4]

REFERENCES

1. J.J. Hoyt and A.A. Potter: *Metall. Mater. Trans. A*, 2012, vol. 43A, pp. 3972–77.
2. E.A. Brandes and G.B. Brook: *Smithells Metals Reference Book*, 7th ed., sections 4–41 and 14–17, Butterworth Heinemann, Oxford, 1992.
3. F. Milstein, J. Zhao, and D. Maroudas: *Phys. Rev. B*, 2004, vol. 70, pp. 184102-1–184102-16.
4. J. Campbell: *Complete Casting Handbook*, Elsevier, Oxford, 2011.

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