Communication

On the Intrinsic Fracture Pressure of Liquid and Solid Aluminum Around Its Melting Temperature

MURAT TIRYAKIOĞLU

To determine the intrinsic fracture pressure of aluminum, data from studies that have used molecular dynamic simulations, the van der Waals method as well as experimental observations have been gathered and analyzed. Results indicate that aluminum has an intrinsic fracture pressure of − 4 GPa at its melting temperature in both liquid and solid states. Moreover, the Fisher equation can be used to estimate the intrinsic fracture pressure of liquid aluminum.

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Hot tears and pores are major casting defects that lead to the rejection of aluminum castings. Although these two defects are quite different in appearance and location, their origin is the same; for both defects, a pore has to first nucleate under a tensile stress, uniaxial for hot tears and hydrostatic for pores. *In situ* observations of hot tear formation in transparent liquids have confirmed[1] the necessity of this first step.

To evaluate hot tear tendencies, there have been several studies to determine the mechanical properties of pure metals and alloys near melting temperature, T_{m}.[2] It is usually assumed that the metal in semisolid or even liquid state is not capable of withstanding tensile stresses. This assumption has been claimed to be validated by experimental results from tensile tests conducted near melting temperatures of pure aluminum and its alloys,[2] which showed the fracture stress (pressure), P_{f}, to be in the vicinity of 1 MPa. An example is provided in Figure 1 by using the data by Pumphrey and Lyons[3] for 99.99 pct pure aluminum. Note that there is a sharp decrease after 650 °C, and the fracture pressure goes down to zero at essentially the melting temperature. Similar results were obtained by Fredriksson *et al.*[4]

It is well known that the necessary condition for the nucleation of a pore in a solidifying liquid, the critical radius above which a pore is stable, r^*, is found by:

$$r^* = \frac{-2\sigma}{\Delta P^*} \qquad [1]$$

where σ is the surface tension of the liquid (N m) and ΔP^* is the pressure differential and is a negative number. Note that while surface tension for liquid metals is known, either ΔP^* or r^* needs to be estimated or alternatively assumed. A review of the literature by Yousefian and Tiryakioğlu[5] showed that ΔP^* is generally assumed to be 1 atm. (0.1 MPa). This is significantly less than the fracture pressure of − 3 GPa calculated by Campbell[6,7] and − 3.4 GPa calculated by Yousefian and Tiryakioğlu.[5] In both studies, ΔP^* was taken as the fracture pressure of aluminum, P_{f}, and the equation developed by Fisher[8,9] based on the classical nucleation theory was used.

$$P_{\mathrm{f}} = -\sqrt{\frac{16\pi\sigma^3}{3kT\ln\left(\frac{kN_{\mathrm{A}}T}{h}\right)}} \qquad [2]$$

where k is the Boltzmann's constant (J K^{-1}), N_{A} is the Avagadro's number, and h is the Planck's constant (J s). It is significant that the ideal tensile strength (fracture pressure) of solid aluminum at the melting temperature was estimated by the Van der Waals method, a completely different approach based on the behavior of gases,[10] to be − 4.8 GPa by Martynyuk.[11]

The calculation of ideal fracture pressure of liquid and solid aluminum at T_{m} was not supported by experimental data reported above. Therefore, another literature survey was conducted to compile data for dynamic fracture testing of solid aluminum at strain rates above 10^6 s^{-1} as these high strain rates provide a "unified approach as non-equilibrium phase transition through formation, growth and coalescence of spherical cavities."[12] At lower strain rates, elasticity of aluminum is expected to suppress spherical voids and micro-cracking should be the general mode of fracture.[12] For liquid aluminum, experiments to generate pressure waves by using femtosecond laser as well as molecular dynamics simulations were reviewed. The details of the data compiled from the literature are provided in Table I. Spall strength data were extrapolated to a strain rate of 10^8 s^{-1} using the empirical equation provided by Kanel.[13]

The complied data as well as the Van der Waals estimated by Martynyuk are presented in Figure 2 as a function of temperature. For solid aluminum, there is a strong agreement between the estimates of Martynyuk, molecular dynamics results and experimental spall strength data at room and melting temperatures. For

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MURAT TIRYAKIOĞLU is with the School of Engineering, University of North Florida, Jacksonville, FL, 32224. Conatct e-mail: m.tiryakioglu@unf.edu

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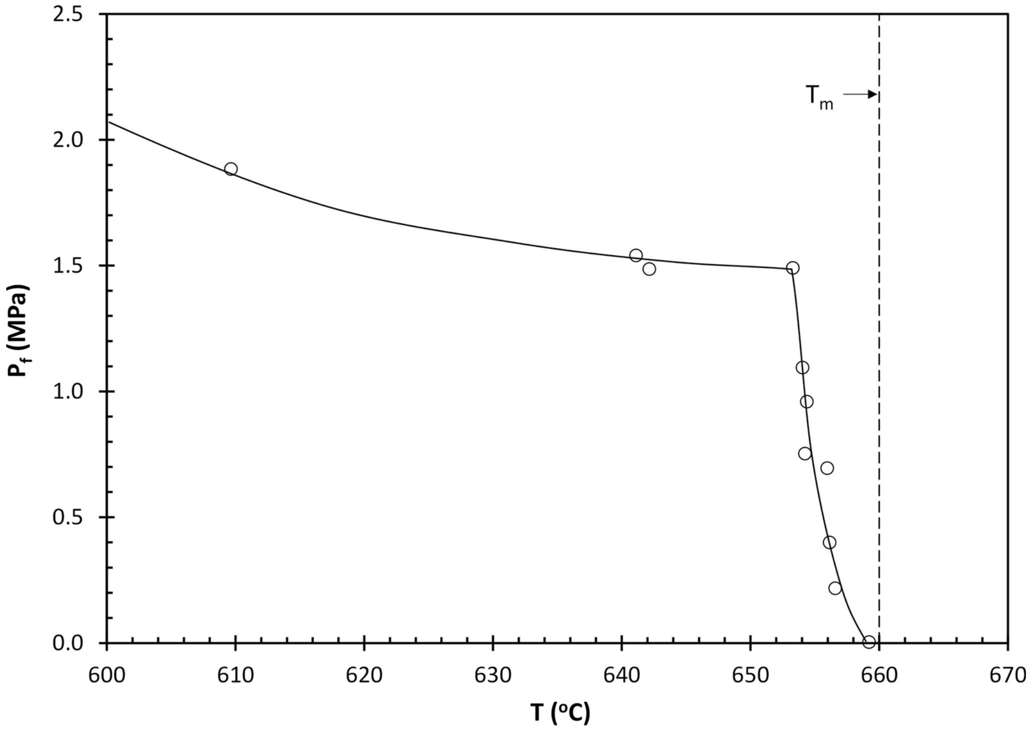

Fig. 1—Fracture pressure results of Pumphrey and Lyons for 99.99 pct pure aluminum.

Table I. Details of the Fracture Pressure Data Compiled from the Literature

Method	References
Experimental (femtosecond laser)	14,15
Molecular dynamics	16 through 19
Experimental (spall strength)	20 through 22

liquid aluminum, femtosecond laser experiments and molecular dynamics simulations are consistent and follow the same trend.

Figure 2 shows that the ideal fracture pressure of aluminum at the melting temperature is approximately − 4 GPa, a value that provides a higher barrier for nucleation of pores than those calculated by Campbell and Yousefian and Tiryakioğlu. Moreover, this value is the same regardless of whether T_m is approached from the solid or liquid side. This result is consistent with the molecular dynamics results of Mayer and Mayer[23] who stated that it was possible to nucleate a pore homogeneously under tension, where the fracture pressure of the melt was comparable to solid aluminum at elevated temperatures.

To determine whether the Fisher equation can be used to estimate the intrinsic fracture pressure of liquid aluminum as a function of temperature, surface tension of aluminum was adjusted by using the equation provided by Lu and Jiang;[24]

$$\sigma = \sigma_m - \delta \cdot (T - T_m) \qquad [3]$$

where σ_m is the surface tension at the melting temperature (N m) and δ is a coefficient (N m/K). Lu and Jiang reported σ_m to be 1.03 N m and δ as 1.5×10^{-4} N m/K. The fracture pressure of liquid aluminum estimated by the Fisher equation is also indicated in Figure 2, which shows that the Fisher equation can be used to estimate the trend of the experimental and molecular dynamics data.

The intrinsic fracture pressure values for liquid aluminum presented in Figure 2 are 3 to 4 orders of magnitude higher than experimental tensile strength values reported in the literature for aluminum alloys at or near their melting temperatures. Consequently, it has been common to assume that there is no energy barrier to nucleation of pores in solidifying metals[25] and that pores are intrinsic defects.[26,27] This discrepancy has been attributed[5,28–30] to the presence of inclusions, namely bifilms, in the solidifying metal, on which pores are nucleated heterogeneously.[5,28,31,32] Hence, bifilms greatly reduce, if not eliminate, the energy barrier for nucleation of pores, resulting in fracture pressure of the solidifying metal to approach zero. If bifilms can be eliminated from aluminum alloys, the intrinsic properties of aluminum are sufficient to overcome many engineering challenges during the production of aluminum castings.

In conclusion, the intrinsic fracture pressure of aluminum at its melting temperature is − 4 GPa, in both liquid and solid states. To estimate the intrinsic fracture pressure of liquid aluminum at a given temperature, the equation developed by Fisher produces reliable estimates. The results of this study indicate that many issues encountered in the production of aluminum castings, such as hot tears and pore formation, are due to extrinsic factors, namely entrainment defects.

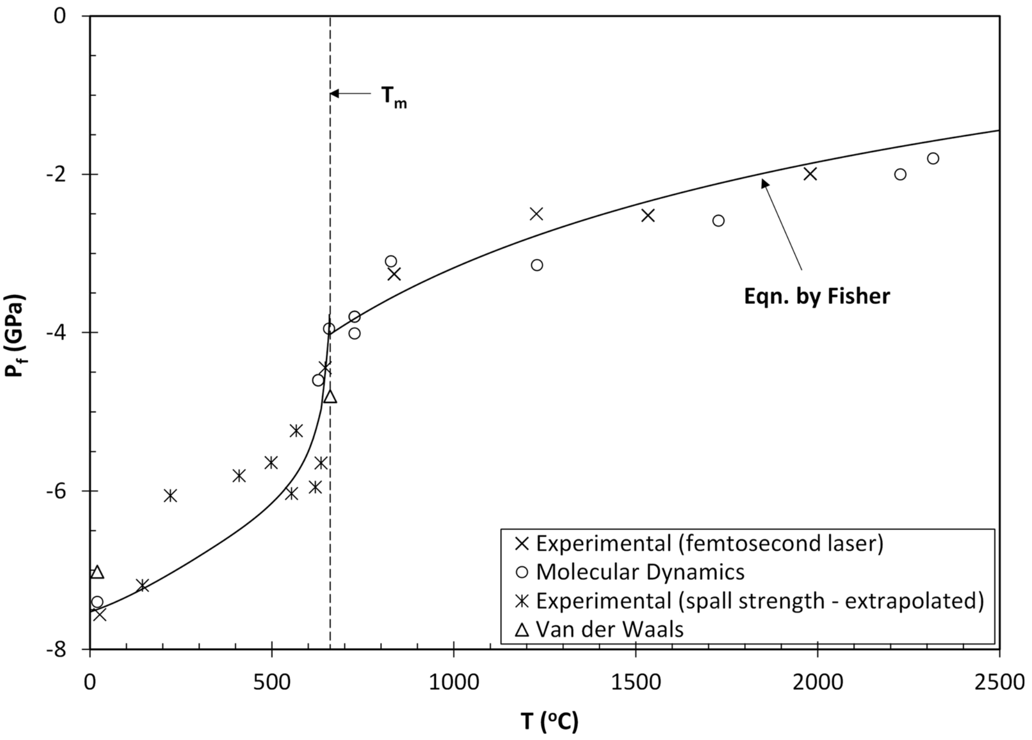

Fig. 2—Change in intrinsic fracture pressure of aluminum as a function of temperature.

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