Comment on "Effect of Impurity Bonding on Grain-Boundary Embrittlement"

In a recent Letter, Goodwin, Needs, and Heine[1] discussed the various models of grain-boundary embrittlement and reported on calculations which were proposed to check several of them. In particular, the authors hoped to determine whether or not the embrittlement was caused by the formation of a weak metal-impurity bond as first proposed by Troiano,[2] or by the formation of a strong bond between the metal and the impurity with a concomitant weakening of metal-metal bonds around the impurity, as first proposed by Losch[3] and elaborated on by Messmer and Briant.[4] The results of their calculations were said to suggest that neither model was correct because they found that cohesion was improved both in the layer of atoms containing the impurity and in the layer adjacent to the one containing the impurity.

Aside from the fact that the atomic arrangement that the authors chose simulated a perfect crystal and not a grain boundary, there is a central flaw to the entire work as it is reported. The calculations were performed for aluminum as the host metal and arsenic and germanium as the segregated impurities. The flaw is that there is no experimental evidence that either of these elements causes embrittlement of aluminum. Consequently, their results do not provide a test as to whether one model or the other is correct. The authors apparently assumed that any segregated impurity causes embrittlement. That is not correct. Boron in nickel and the intermetallic compound Ni_3Al and carbon in iron and steel both improve cohesion when they segregate to the grain boundaries.[5] Other impurities such as sulfur in nickel and iron and antimony in nickel and iron cause embrittlement. Table I lists all well documented cases of impurity-induced embrittlement. If one is to check various theories of impurity-induced embrittlement, it is of great importance to perform calculations on one of these systems where one can assume that changes in bonding *could* contribute to the embrittlement. Otherwise, the results such as those obtained by Goodwin, Needs, and Heine are meaningless.

C. L. Briant
Research and Development Center
General Electric Company
Schenectady, New York 12301

K. Sieradzki
Department of Materials Science
The Johns Hopkins University
Baltimore, Maryland 21218

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TABLE I. Cases of impurity-induced embrittlement.

Host element	Embrittling element	References
Cu	Bi	Hondros and McLean (Ref. 6)
Cu	Te	Marcus and Paton (Ref. 7)
Fe	S	Jolly and Goux; Pichard, Rieu, and Goux; and Ramasubramanian and Stein (Refs. 8–10)
Fe	P	Ramasubramanian and Stein (Ref. 10)
Fe	N	Hopkins and Tipler (Ref. 11)
Fe	Sn	Seah and Hondros (Ref. 12)
Fe	Te	Rellick *et al.* (Ref. 13) and Pichard, Rieu, and Goux (Ref. 9)
Fe	Se	Pichard, Rieu, and Goux (Ref. 9)
Mo	O	Touboul, Minel, and Langeron (Ref. 14)
Ni	S	Lozinskiy, Volkogon, and Pertsovskiy; Thompson; and Holt and Wallace (Refs. 15–17)
Ni	Sb	Bruemmer *et al.* (Ref. 18)

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