MATDAT18: Materials and Data Science Hackathon

Team Composition (2 people max.)

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Project Title

Mitigating Hazards Posed by Stretchable Electronic Circuits: Liquid Metal Embrittlement by Exposure of Engineering Alloys to Eutectic Gallium Indium

Project Synopsis (approx. 100 words)

Liquid metal circuitry is a potentially transformative technology that promises to enable flexible, stretchable and self-healing electronics for applications including wearables, e-textiles, and soft robotics. However, under some conditions liquid metals can cause catastrophic brittle failure when they contact solid metals, a phenomenon called liquid metal embrittlement (LME). Currently, no data exists on the embrittling effects of the liquid of interest in these circuits. As a result, a comprehensive test matrix is impossibly large; however, 70 years of data exists for related systems exhibiting LME. The objective of this project is a data-driven experimental design, specifically seeking to identify the likely variables and combinations thereof with importance for LME in the systems of interest.

Identified Data-Science Collaborative Need (approx. 100 words)

The number of variables investigated in previous studies of liquid metal embrittlement is large: crystallite orientation, crystallite size, temperature, loading rate, stress state, exposure time, pre-loading, chemical compositions, etc. While general trends exist for severity of embrittlement with most of these variables, most examples in the literature are accompanied by exceptions under modified conditions. Decades of human intuition have utterly failed to extract relationships between the variables of interest, likely because no strong single-variable relationship dominates behavior. A blindly constructed experimental test matrix of sufficient complexity to unravel interdependencies is unreasonably large. Using existing data primarily extracted from the literature, it is anticipated that a data-science collaboration would facilitate development of a more tractable experimental test matrix, ultimately enabling identification of the most promising strategies for mitigation of embrittlement.

Data Origin and Access (*data must be available and sharable with data science teams* – please address: data source/origin, access privileges, sharing privileges)

Data has been mined by my graduate student from hundreds of published papers, many of which have been digitized for the first time. Additional data will be produced from experiments in my laboratory in the next 2-3 months.

The data for this project will be fully shareable and publishable (with appropriate attribution).

Project Description (approx. 1.5 pages, plus figures and references; please describe data size, form, dimensionality, uncertainties, number of examples, etc.)

Newly developed flexible and reconfigurable circuit technology based on liquid metal alloys are potentially transformative in both military and commercial applications as on-the-fly reconfigurable antennas, flexible connections, and sensors [1]. However, liquid metals are known to cause severe embrittlement in normally ductile metals, leading to catastrophic failure as shown in Figure 1. The only requirement for failure in susceptible metals is a small amount of surface contact, such as what would be necessary for electrical conductivity in a circuit bearing these materials. Other metal components of these liquid metal electronics may be vulnerable to the liquid metals and, following failure of the device, surrounding structural components could also be exposed. The proposed project will use data extracted from the literature to identify testing conditions most likely to produce embrittlement and identify experimental variables which may enable the development of mitigation strategies.

The liquid metal alloy that has received the most attention for flexible circuit applications is a gallium-indium mixture called eGaIn, but no experimental data currently exists on the effects of eGaIn on any engineering alloy. Past work has not deduced a definitive cause of liquid metal embrittlement (LME), and no model currently exists to predict if embrittlement will occur under a given set of experimental conditions [2]. The only currently available method to determine the behavior of a solid metal in a particular liquid metal environment is Edisonian experimentation. However, at least 70 years of literature and data on the LME process exists in other related systems [3].

Developing sufficient understanding of the effects of eGaIn on engineering materials via experiment alone is intractable, but this understanding is necessary before eGaIn devices can be widely implemented. Virtually every experimental variable ever tested has been shown to have a possible effect on the occurrence and severity of LME, and human intuition has failed to extract relationships that dominate behavior [4], [5]. *The objective of this project is the development of data-driven experimental test matrices targeting: a) engineering alloy classes most likely susceptible to embrittlement and b) potential material modifications likely to mitigate the severity of LME.*

To this end, a PhD student has conducted an extensive literature review of known cases of LME. Like many data-centered problems in materials science, LME suffers from a relatively small data pool (10^2 –10^3 unique quantified experiments) due to the time and cost of each additional data point. Data has been extracted from hundreds of papers (e.g. Figure 1 [6]), many of which have never before been digitized. Approximately fifteen experimental variables were captured (if reported) for each experiment, plus the elemental composition of the liquid and the solid. These variables were either quantified or broken into distinct classes and are currently stored as a spreadsheet.

An additional challenge arises from the lack of a standardized metric by which “embrittlement” is measured. Two proposed metrics quantifying the severity of embrittlement are proposed and calculated for each recorded data point, enabling the comparison of data from different authors.

In the short term (2-3 months), Miller's laboratory will conduct a small number of LME experiments (approximately 10) with eGaIn. These experiments are necessary to establish standard handling and testing protocols for these materials, but they have the added benefit of adding some fully characterized eGaIn data points to the data extracted from the literature.

It is the opinion of the authors that the historical failure to understand the LME phenomenon is at least partially due to the assumption of "specificity," where embrittlement is considered a binary value for any given liquid-solid pair (e.g. liquid In will embrittle all Al alloys but no Mg alloys). This view of LME was first described by Rostoker in 1960 [7], and the assumption of specificity heavily influenced subsequent literature. As a result, many combinations of liquid-solid combinations were deemed "embrittling" or "non-embrittling" based on a single experiment, disregarding other variables that are of demonstrated importance, e.g. temperature (Table 1) [2]. It is likely that, under modestly modified experimental conditions, many of these systems could demonstrate some level of embrittlement.

<u>A more nuanced analysis of the available data is necessary, and a partnership with a data science team will directly enable this analysis</u>. With guidance from the historical literature, a manageable experimental test matrix can be identified, focusing on the identification of the solid alloys that pose greatest potential hazards and the development of LME mitigation strategies through material modification. This targeted experimental characterization enables both further development of liquid metal circuitry, as well as a greater scientific understanding of the poorly understood liquid metal embrittlement phenomenon.

Figure 1. Liquid metal embrittlement by gallium metal on an aluminum soda can.

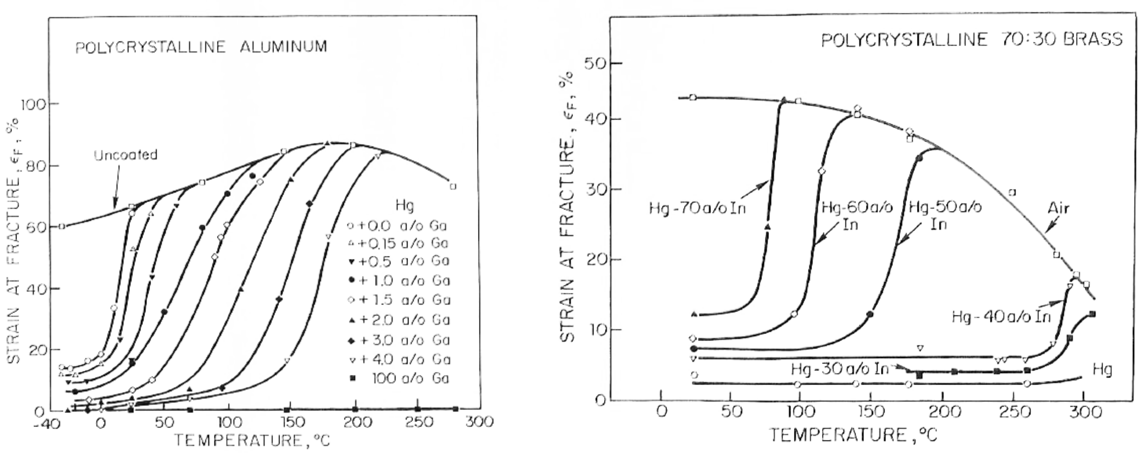

Figure 2. Example data on the variation of embrittlement with temperature and composition of the liquid for two different solid metals. Data from each plot was digitized and recorded [4].

Table 1: Summary of reported non-embrittling couples, illustrating that the behavior of entire classes of alloys has frequently been inferred from a single test [2].

Summary of Non-Embrittling Couples

P - element (nominally pure)
A - alloy
C - commercial
L - laboratory

a - limited testing (known or inferred)
b - one test temperature (inferred)
c - no published information on test
e - also reported as embrittling

Solid \ Liquid		Hg		Ga	Na	In	Li	Se	Sn	Bi	Tl	Cd	Pb	Zn	Te
		P	A	P	P	P	P	P	P	P	P	P	P	P	P
Bi	P			c											
Cd	P	a	a												
Pb	P	c													
Zn	P												c,e		
Mg	CA		b	b		b	b	b	b	b	b	b	b		
Al	P								a						
	CA						b	b		b	b	b	b		
Au	P	b		b											
Cu	CP	c,e		c					c					c	
Fe	P	b	b			b									
	LA	b	b												
	CA		b	b	b			b	b,e	b	b		b,e		
Ti	CA			b	b	b	b	b	b	b	b		b	b	b

[1] M. D. Dickey, “Stretchable and Soft Electronics using Liquid Metals,” *Advanced Materials*, vol. 29, no. 27, p. 1606425, Jul. 2017.
[2] F. A. Shunk and W. R. Warke, “Specificity as an aspect of liquid metal embrittlement,” *Scripta Metallurgica*, vol. 8, no. 5, pp. 519–526, 1974.
[3] A. R. Westwood, C. M. Preece, and M. H. Kamdar, “Adsorption-Induced Brittle Fracture in Liquid Metal Environments,” MARTIN MARIETTA CORP BALTIMORE MD RESEARCH INST FOR ADVANCED STUDIES, No. RIAS-TR-67-8C., 1967.
[4] M. G. Nicholas and C. F. Old, “Review: Liquid Metal Embrittlement,” *Journal of Materials Science*, vol. 14, pp. 1–18, 1979.
[5] Kamdar, Madhusudan H., “Liquid Metal Embrittlement,” in *Embrittlement of Engineering Alloys*, vol. 25, New York: Academic Press, Inc., 1983.
[6] C. M. Preece and A. R. Westwood, “Temperature-Sensitive Embrittlement of FCC Metals by Liquid Metal Solutions,” *Transactions of the American Society for Metals*, vol. 62, p. 418, 1969.
[7] W. Rostoker, *Embrittlement by liquid metals*. Reinhold Publishing Corporation, 1960.