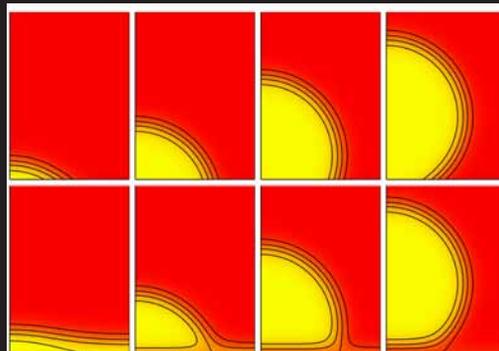


Metrics for Reactive Wetting in Complex Systems

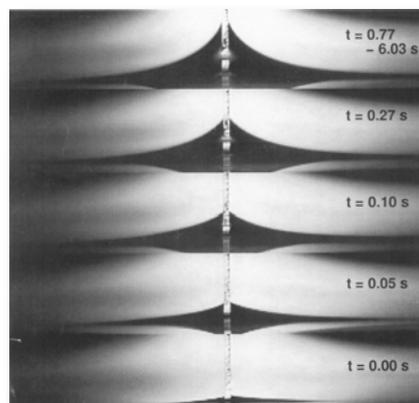
Objective

For processes involving wetting between two materials, classically defined metrics such as surface or interface energy and contact angle are only a starting point for understanding the dynamic behavior of complex or nanometer-scaled systems that involve chemical reaction/diffusion. The goal of this work is to have a quantitative model of reactive wetting. A good model should allow correct interpretation of dynamic measurements such as the wetting balance (a standard in solderability tests) and the meaning of contact angle measurement of systems not at equilibrium. Tools must also be developed to disseminate these results as codes usable by others.



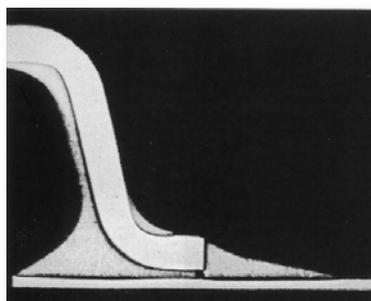
Impact and Customers

- A measurement need as stated in the IPC (Institute for Interconnecting and Packaging Electronic Circuits) report is the development of tests that properly capture how solder wets a printed wiring board, and to predict the service performance of the formed joint.
- Models of this behavior should allow modifications to the widely used wetting balance test, with the goal of eliminating errors and extracting data more useful for solder joint design.
- Additional areas of potential impact are found in nanofabrication with processes such as the controlled breakup of thin film deposits to form nanoscale droplets, or the growth of nanowires by the vapor-liquid-solid (VLS) method. These processes are encompassed by our theory, as the surfaces, interfaces and triple junctions of a three phase system are treated quite generally.



Approach

From fundamental physical considerations, we have derived a set of partial differential equations describing wetting and spreading. These equations are derived using a variational thermodynamic principle applied to a two component alloy system with three (vapor, liquid and solid) phases. The method naturally includes time dependent chemical interactions between substrate and liquid and also non-classical (diffuse interface) effects. The latter are important for applications where the system size approaches nanometer dimensions.



Numerical solution of the equations will be performed for specific wetting geometries and parameter values. Results will be compared to predictions of simpler theories and experimental results. The importance of solute transport and its influence on the surface energy will be examined. A sensitivity analysis will determine those factors that dominate the wetting process. We will use the model to determine how to interpret the measurements of the wetting balance to best aid in the design of solder joints for fine pitch electronics. Subsequently, these tools will be applied to thin film breakup, heterogeneous nucleation on shaped particles, and VLS nanowire growth.

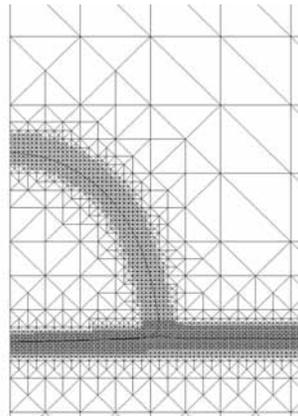
Accomplishments

We have implemented a numerical solution scheme to solve these equations and are examining the predictions. Four coupled partial differential equations comprise the model: a mass balance equation, a modified Navier-Stokes equation for the velocity of the matter in the various phases, a modified diffusion equation for the concentration field, and an equation to treat the dynamics of the solid-fluid interfaces (phase field). Solving this system of coupled equations accurately with appropriate parameters requires sophisticated numerical solution techniques and long simulation times. Our approach thus far has yielded a complete solution of the equations in two dimensions with a slightly unrealistic parameter set to enable the solution of the equations in a practical time frame.

An adaptive mesh is being used to solve the differential equations. A fine mesh is needed near the three interfaces between the liquid, solid and vapor for the spreading drop problem in order to have the numerical accuracy necessary to maintain correct changes in concentration across interfaces. The mesh moves (adapts) as the droplet spreads and the solid is partially dissolved. Only a coarse mesh is needed in the interior regions of the liquid, solid and vapor phases because gradients are less severe there.

A plot of contact angle (θ) versus triple junction speed (capillary number, Ca^*) shows a large contact angle at high speed that decays to the equilibrium contact angle as the triple junction slows down to zero

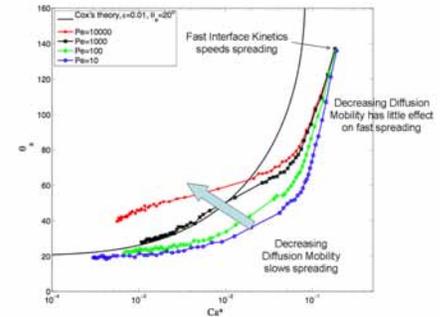
when spreading is complete. The general shape of the curve is known from fluid mechanics analysis and measurements for nonreacting cases (solid curve). In the model, this limit has been recovered numerically by setting solute diffusion and interface mobility parameters to zero. This confirms the validity of the model. For non-zero values of these parameters, the contact angle versus triple line speed curve is altered. The wetting is generally faster than the fluid mechanics case when phase change and diffusion are allowed.



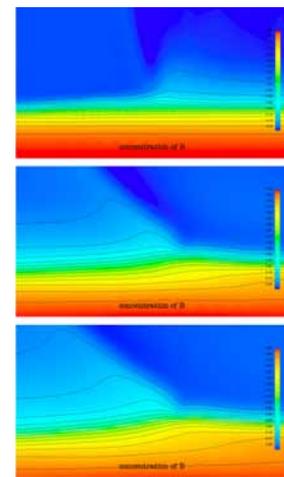
Adaptive mesh used for numerical computation.

Fine scale details of the concentrations near the moving triple line are also being examined. The changing concentrations near the triple line change the local values of the surface energies and affect the contact angle. The top figure (large contact angle and high speed) at the early stage of spreading shows a relatively uniform liquid concentration with an altered vapor

concentration in front of the moving liquid droplet. At later stages (bottom figure), the concentration gradients exist mostly in the liquid and solid.



Contact angle (θ) vs. triple junction speed (Ca^*).



Enlarged view of concentration field near the moving triple junction at three times.

Learn More

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Publications

Moon KW, Boettinger WJ, Williams ME, Josell D, Murray B, Carter WC and Handwerker CA *Dynamic Aspects of Wetting Balance Tests* J. Electronic Packaging, 118: 174 (1996)

Warren JA, Boettinger WJ and Roosen AR *Modeling Reactive Wetting* Acta Materialia, 96: 3247 (1998)

Granasy L, Pusztai T, Saylor D and Warren JA *Phase-field Theory of Heterogeneous Crystal Nucleation* Physical Review Letters, 98 (3): 035703 (2007)

Warren JA, Pusztai T, Környei L and Gránásy L *Phase Field Approach to Heterogeneous Crystal Nucleation in Alloys* Phys. Rev. B, 79: 014204 (2009)