SAND2010-8462C

Coupled Thermo/Hydro Dynamic Models of High Temperature Interface Evolution

Frank van Swol (1814)

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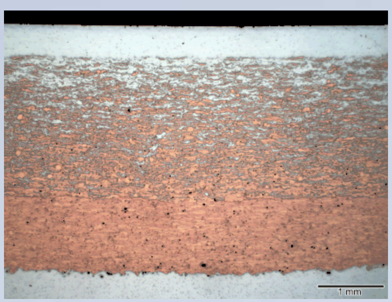
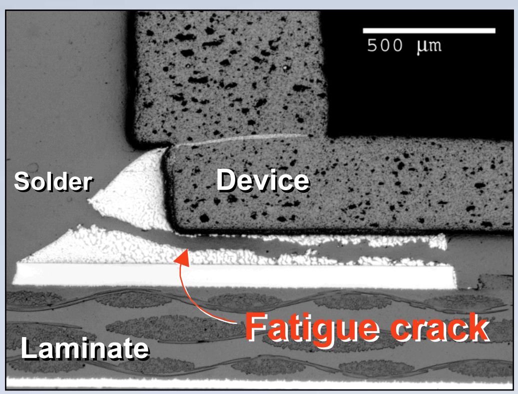
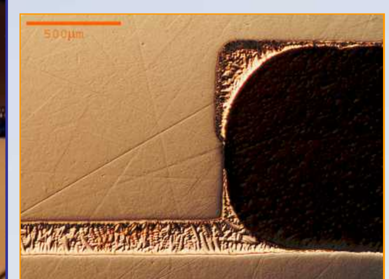
The Problem: Reactive Wetting and Spreading

- **Reactive wetting and solidification are critical to interface formation in soldered, brazed, and welded joints, along with thermal spray coatings**

- **Continuum models of interface are needed to**
  - Improve fundamental understanding
  - Predict/enhance interface performance & reliability



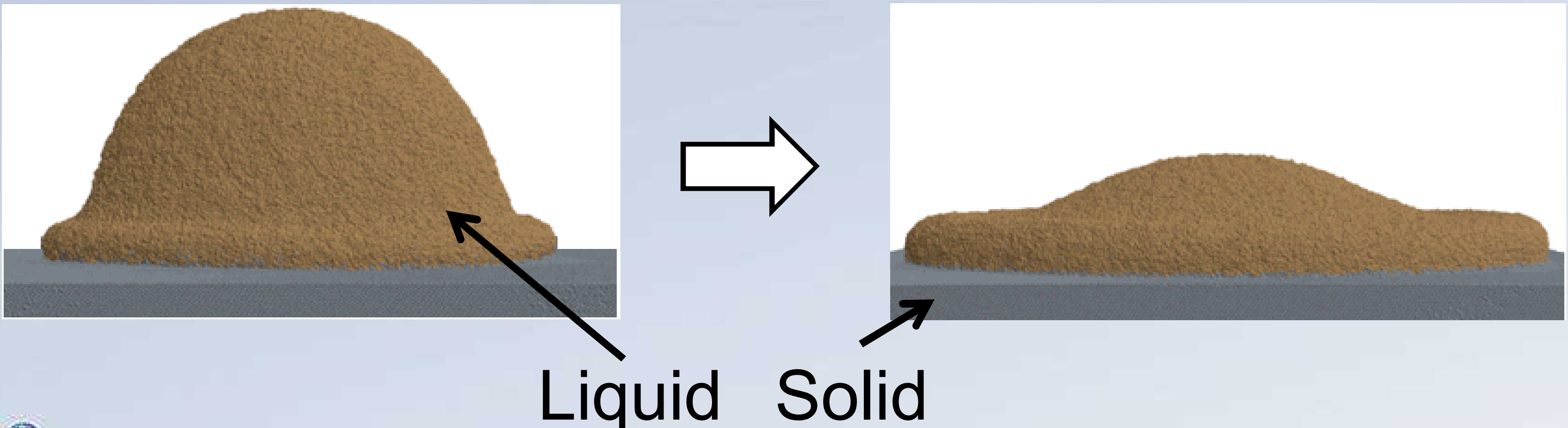




Continuum Model Challenges

Reactive interface problem combines:

- **Large gradients (temperature, velocity, etc.)**
- **Moving boundaries**
- **Chemical-dependent boundary conditions**
- **Nonequilibrium thermodynamics**



Courtesy E.B. Webb III (2010)

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Continuum Model Challenges

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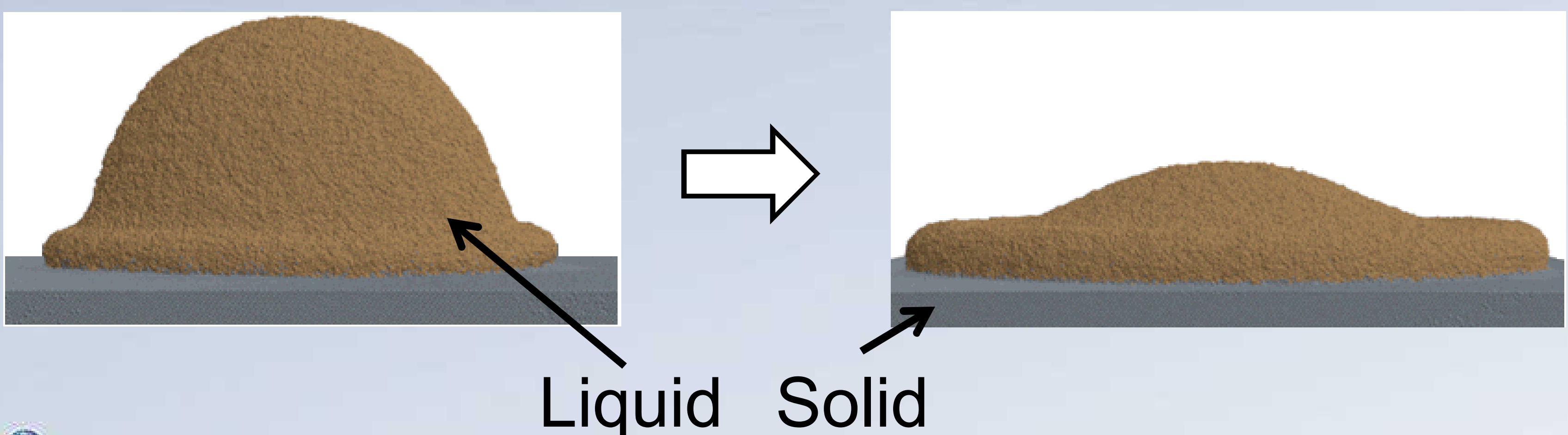
} Need Molecular Dynamics (MD) Simulations



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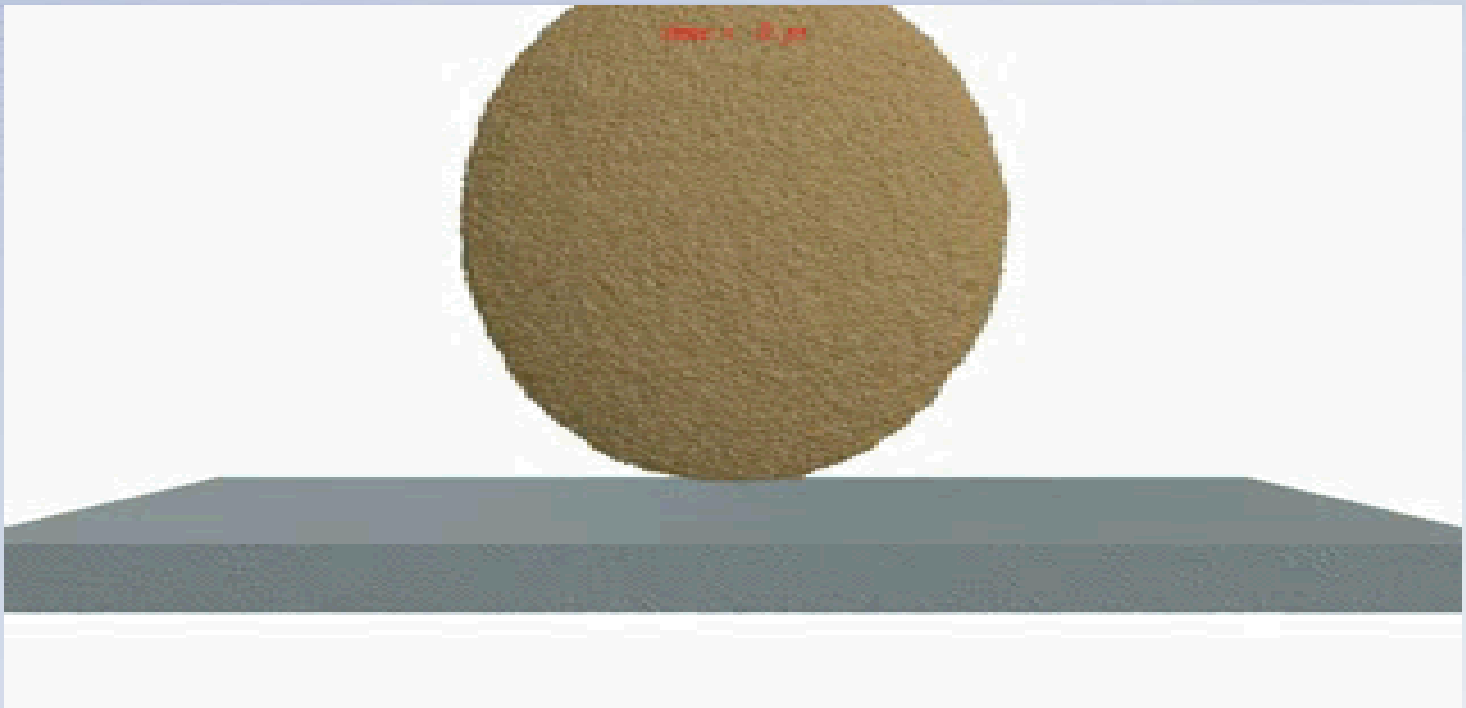
MD State of the Art

- **Recent MD simulations can accurately reproduce experimental droplet impact behavior**
  - MD can model the same dimensionless Weber #s as experiments
  - Same velocity and diameter dependence found between simulations and experiments
- **With MD, atom populations can provide detail and resolution of droplet and substrate physics not previously possible**

MD Simulation

- **50 nm Cu droplet onto Pb (111) Solid Surface**
  v_d = 400 m/s T_{cu} = 2500 K T_{Pb} = 300 K $N_{atom} \sim 40x10^6$



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MD Simulation

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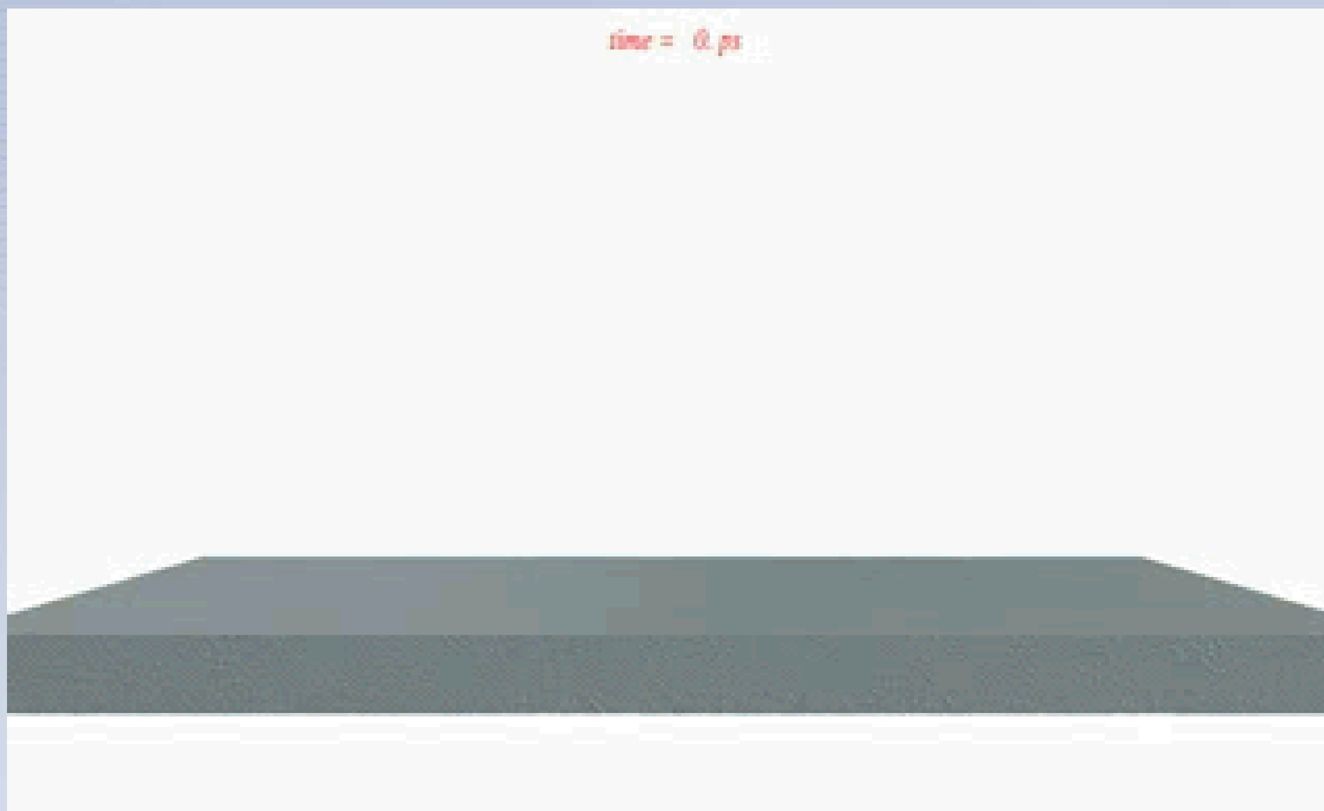

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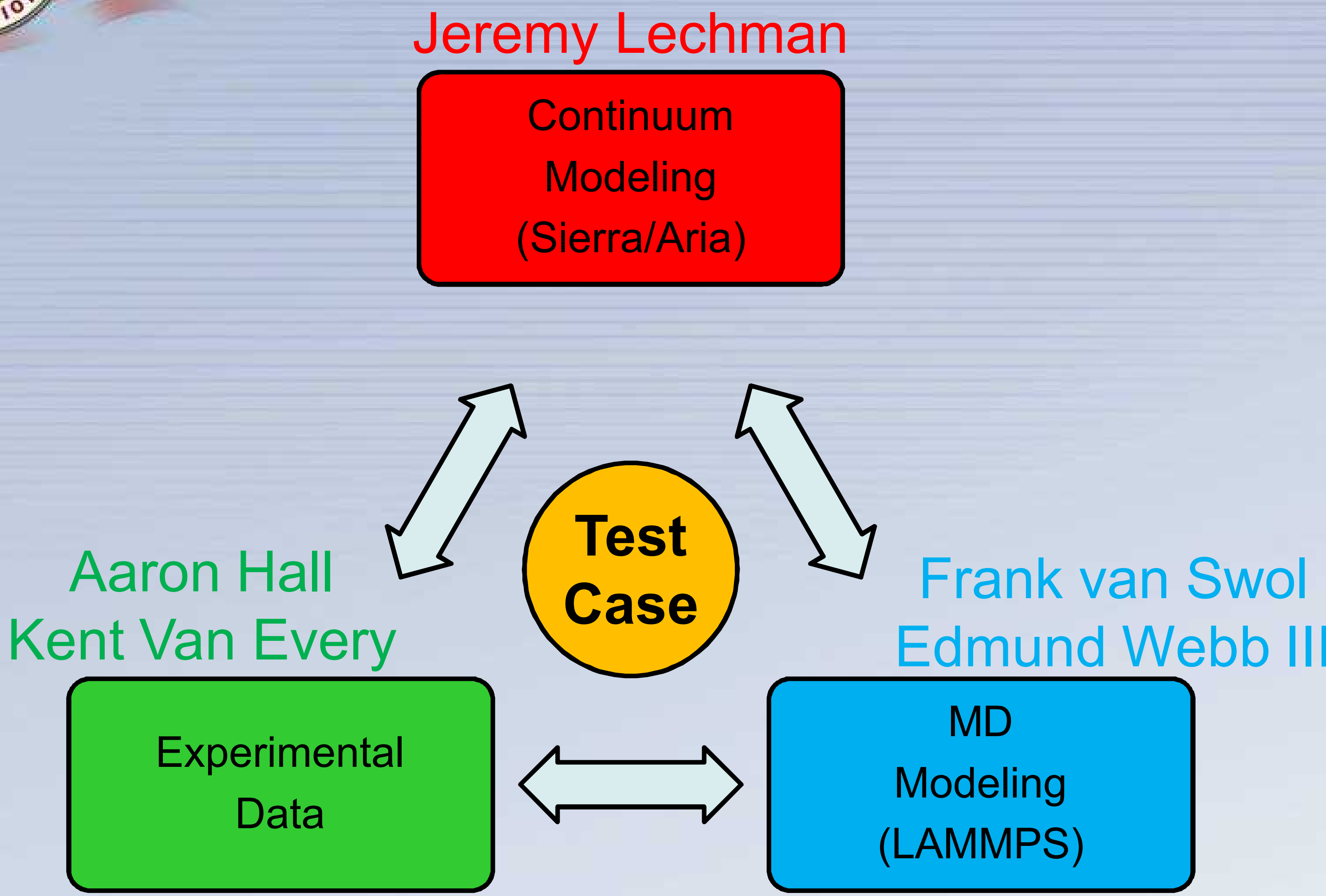
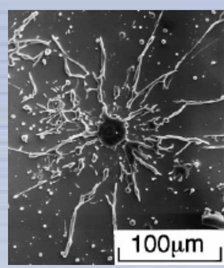
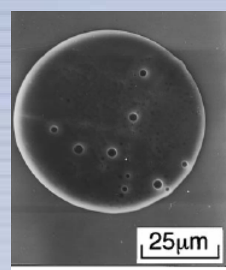
Project Approach

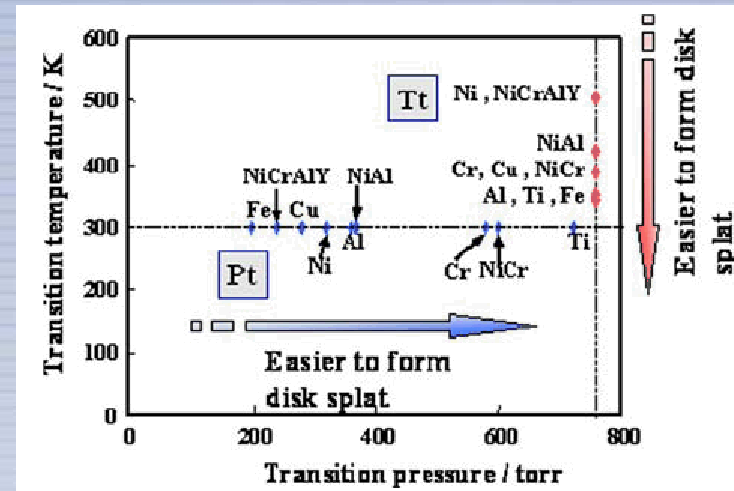


Archetypical Test Case

- **Droplet impacting on a solid surface**
  - Model splash-to-disk transition

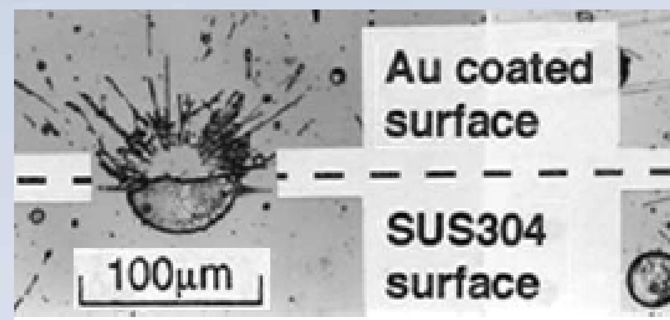






- **Transition behavior depends on:**

  P_{amb}, T_{sub}, γ, p_d, t_{solid}, …



- **Applicability to joining**
  - γ governs solder joint shape
  - Heat transfer during arc welding depends upon p_d
  - P_{amb} can alter weld pool surface

Y. Tanaka, *Surf. Coat Tech.*, 120-121 (1999)
Fukumoto, *J. Therm. Spray Tech.*, 16 (2007)

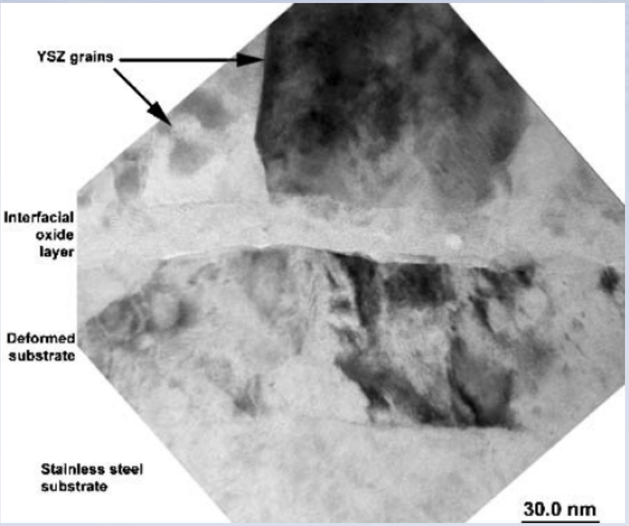
Thermal Spraying vs. Joining Process

- **Droplet conditions are better controlled in a thermal spray process**
- **A wider range of droplet conditions are possible with thermal spraying**
  - Droplet velocity range: 50 – 500 m/s
  - Droplet temperature range: 100 – 3500°C
- **A wider range of droplet and substrate compositions are possible with thermal spraying**

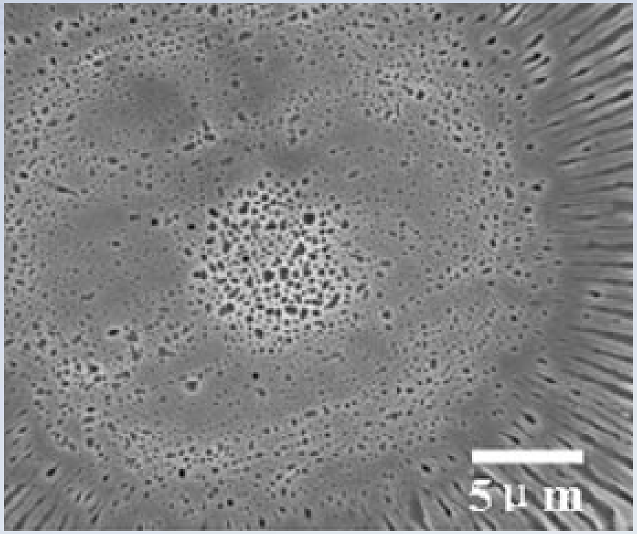
Experimental Data for Simulations

- **Determine splash/disk regimes for Cu splats on Cu plate**
  - Deposit droplets via air plasma spray
  - Measure D_d, T_d, and v_d @ impact

  } Current TSRL capabilities
- **Splat & splat – substrate interface characterization**
  - Composition gradient
  - Grain structure
  - Porosity
  - Shape



TEM of splat-substrate interface

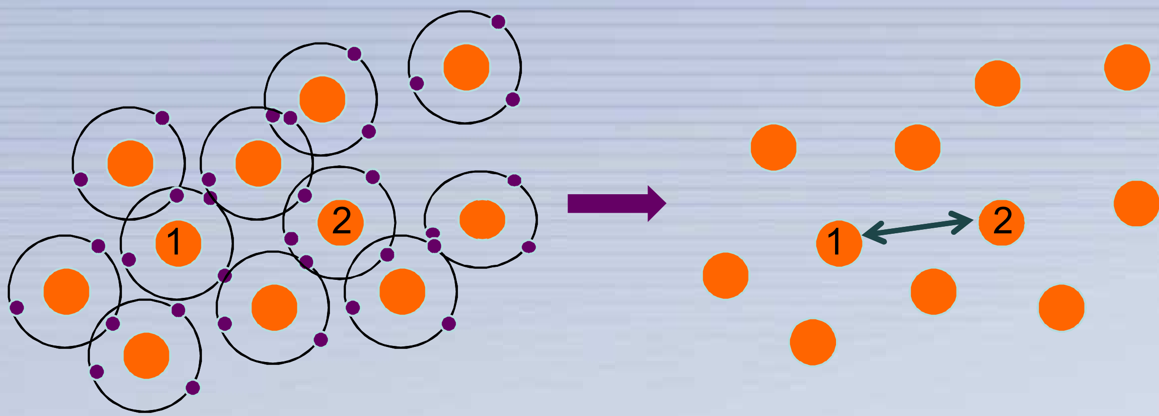


SEM of splat bottom

Fauchais, *J. Therm. Spray Tech.*, 18 (2009)   Yang, *J. Therm. Spray Tech.*, 18 (2009)

Required MD Development

Limitation: Embedded Atom Method (EAM) integrates out electronic degrees of freedom

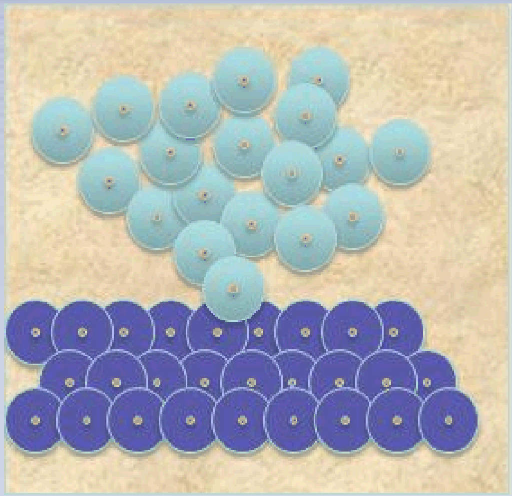


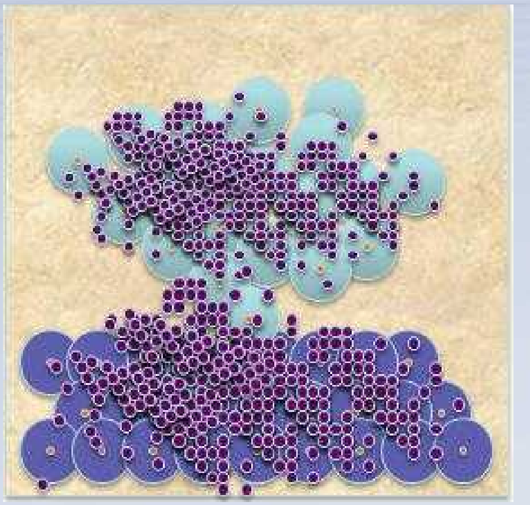
- Thermodynamics & metal ion dynamics captured in "atom" potentials
- Contribution of electrons to conduction is lost

Enabling Electronic Conductivity

Novel Multiparticle Collision Dynamics (MPCD) Approach

- Integrate into LAMMPS a fluctuating background thermal fluid bound to metal ions
- Perform local "collisions" to update background fluid



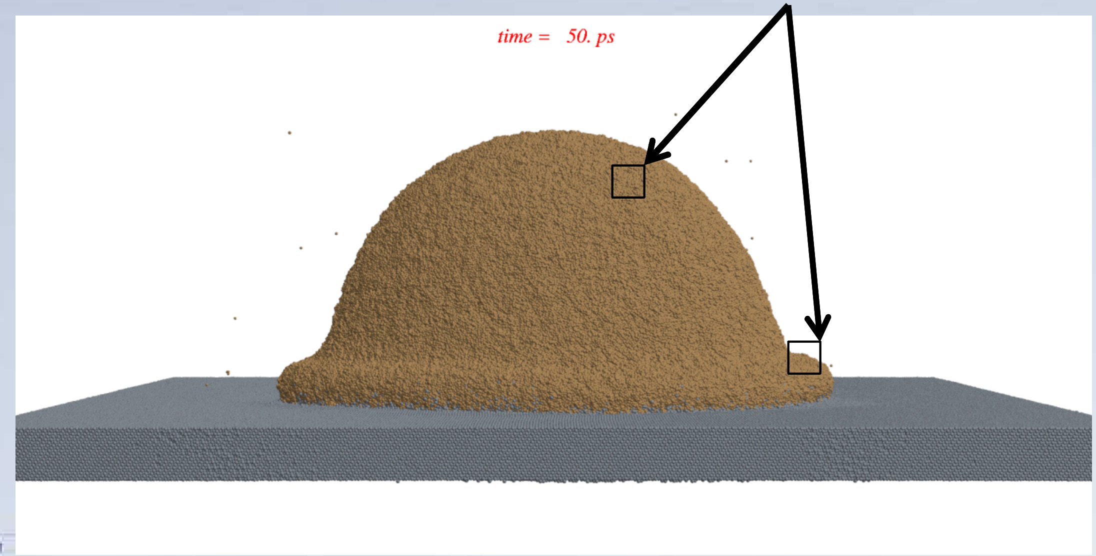


Advantage: Reflects local, strongly varying electron density.

3. The Problems

Connecting MD and continuum example

$$P_l - P_v = \frac{2\gamma}{R_{curv}}$$



independently measure

$$\frac{2}{R_{curv}} = \frac{1}{R_x} + \frac{1}{R_y}$$

and

$$P_l - P_v$$

3. The Problems

Reactive Wetting is a chemical boundary condition

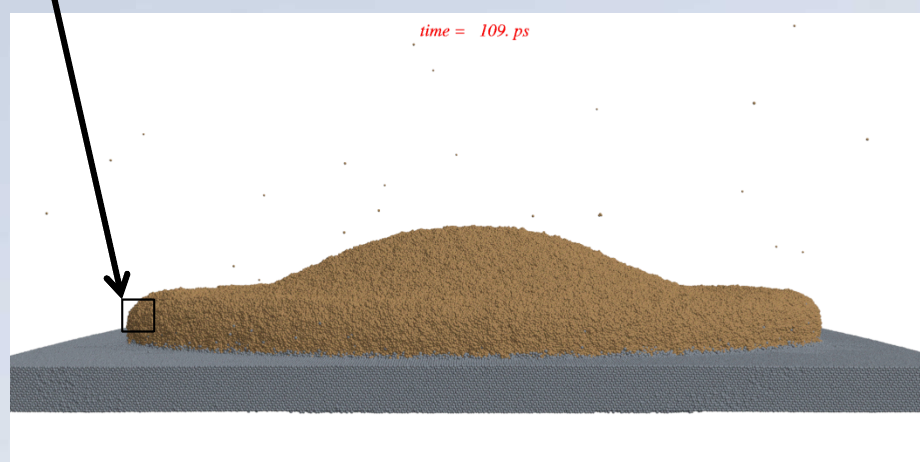
equilibrium

$$\cos\theta = \frac{\gamma_{SL} - \gamma_{SV}}{\gamma_{LV}}$$

$$\gamma_{SL} = \gamma_{SL}(x)$$

$$\therefore \quad \theta = \theta(x)$$

(bulk)
equilibrium
composition



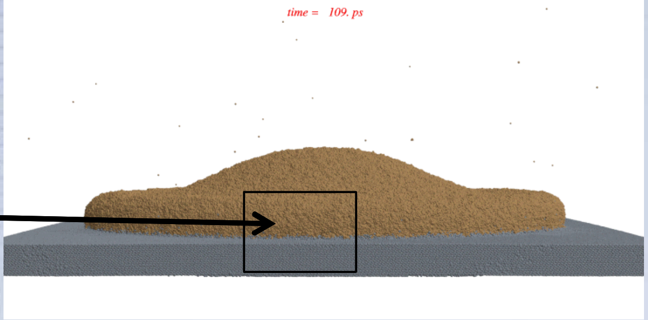
3. The Problems

Solid-liquid interface is generally not at equilibrium

conclude: SL surface free energy is a functional of the local composition profile

$$\gamma_{SL} = \gamma_{SL}\left[x(\mathbf{r})\right] \quad \Rightarrow \quad \theta = \theta\left[x(\mathbf{r})\right]$$

composition profile



Novel solution: two-step approach to obtaining $\gamma_{SL}\left[x(\mathbf{r})\right]$

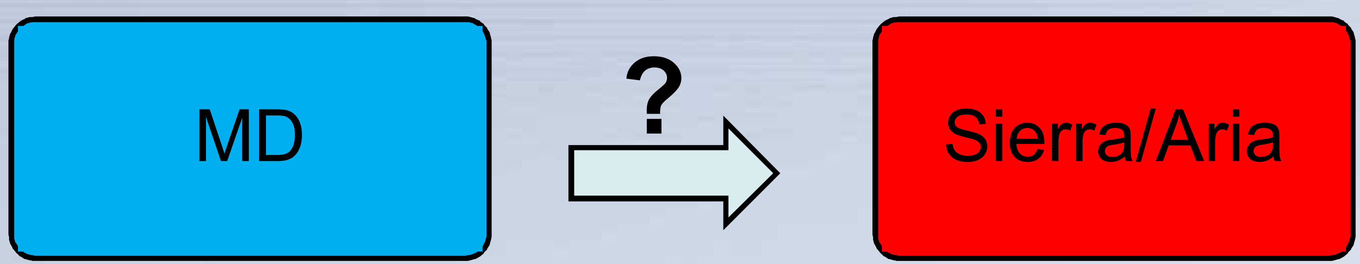
1. obtain profile $x(\mathbf{r})$ from MD
2. generate γ_{SL} from $x(\mathbf{r})$ with constrained fluids density functional theory (DFT)

(Note, DFT for EAM potentials is a new idea)

Linking MD and Continuum Models

Solid-liquid (SL) interface is generally not at equilibrium

$\therefore$ **SL surface free energy (γ_{SL}) is a function of the local composition profile, x(r)**



- Provides x(r)
- γ_{SL} hard to obtain

- Needs γ_{SL} to calculate wetting contact angle

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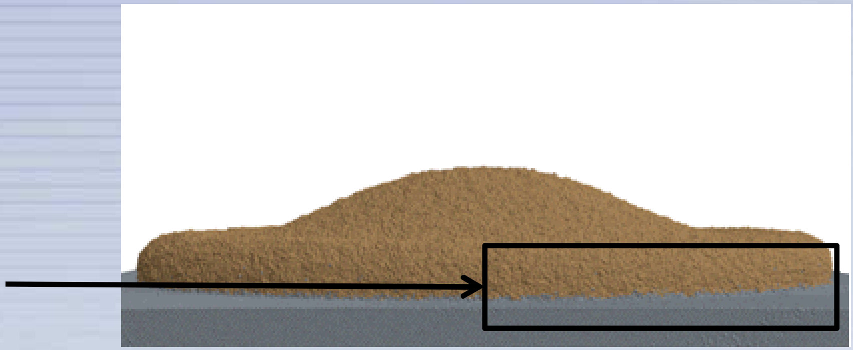
Linking MD and Continuum Models

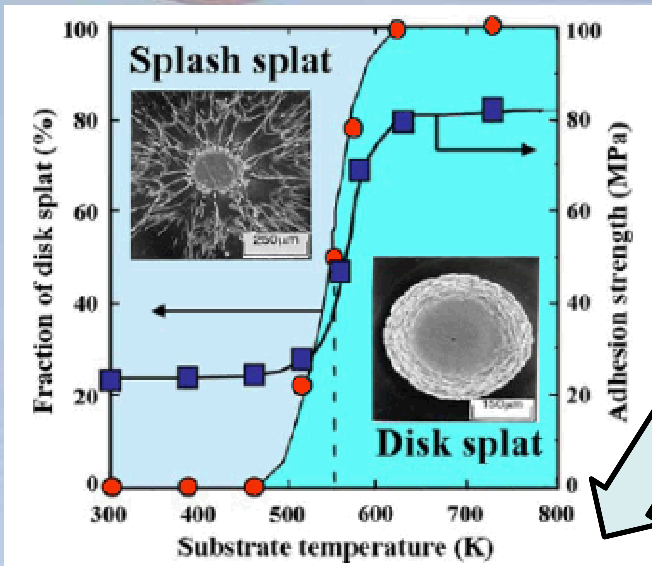
<u>Novel</u> Approach to Obtaining $\gamma_{SL}[x(r)]$

1. Obtain profile composition profile, x(r), from MD



2. Utilize constrained fluids density functional theory (DFT) in Tramonto code to calculate γ_{SL} directly from x(r)

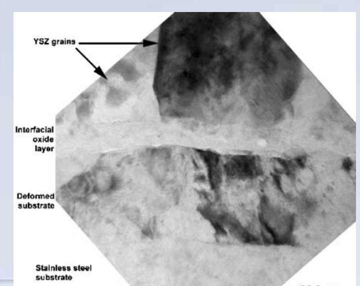
Summary



Continuum Modeling

Experimental Data

MD Modeling



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Milestones

- Determine splash and disk temperature regimes for Cu splats on Cu plates
- Utilize MD droplet simulations to reproduce Cu on Cu splash to disk transition behavior
- Evaluate capabilities of current continuum codes to model the test case
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