# Application of MD (molecular dynamics) methodology in the development and verification of advanced MEMS materials for future wafer probe cards

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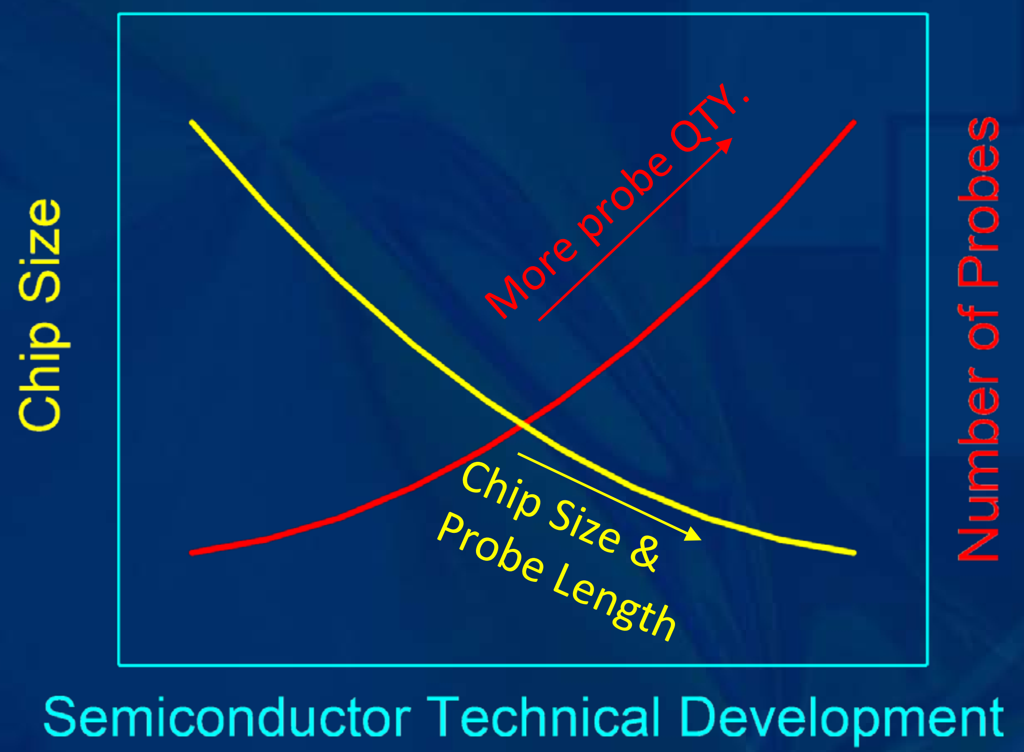
# Overview

- Needs of new materials for the probes in a probe card
- Brief introduction of simulation hierarchy
- Molecular dynamics (MD) simulation
  - ✓ Conventional methods to measure materials properties
  - ✓ Importance of simulation methodology in predicting the materials properties
  - ✓ Data processing for crystal defect and density functional theory (DFT) simulation
- Cognitive simulation with a real MEMS Probe
  - ✓ Mechanical data and Multi-physical (Mech/Elec/Ther) data
  - ✓ Analysis of the gaps between simulation and measurement data
- Summary
- Future works

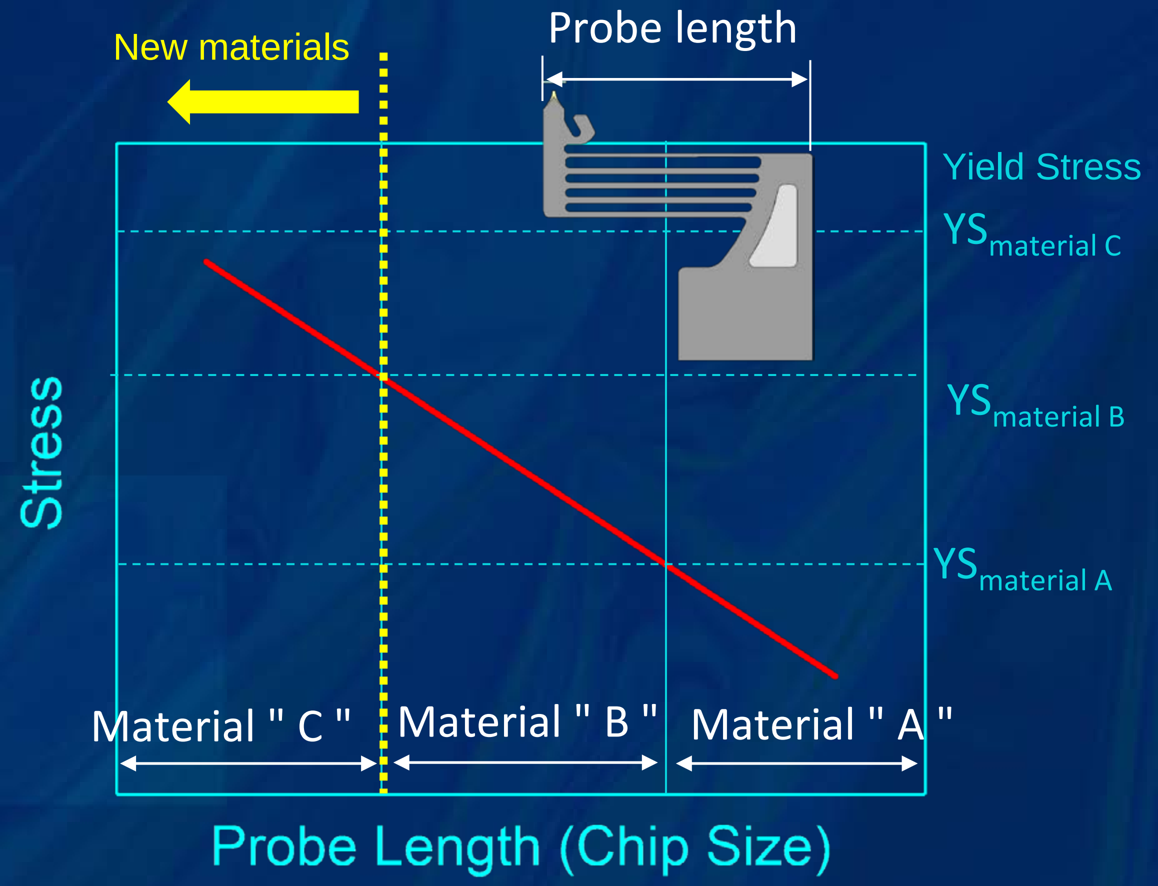
# Objective of our study with a simulation hierarchy

# Trend of chip size and the number of probes in a wafer

- **Smaller chip size links to shorter probe length, which in turn necessitates the development of new materials with unique properties**



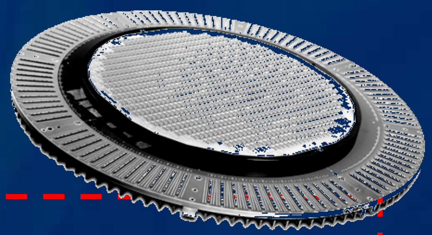

✓ **Trend of chip size vs. the number of probes**




✓ **Requirement of probe length vs. yield stress**

# Simulations hierarchy from materials to systems

- Technical level of simulations to help develop new probes



" What is the level 0? "

Level 0

Materials properties

Digital twin : " Real world = Simulation world "

Level 1

- 3D Modeling & analysis
- Structure simulation

Level 2

- Test data matching
- Multi-physics simulation

- CAE Model
- Test result data

Level 3

- Analysis / Prediction
- Structure Optimization

A.I. study

Deep learning

Machine learning

# Process of
# Molecular Dynamic (MD)
# Simulation

# Evaluation of materials properties by conventional methods

- **Tensile test**
  - ✓ The most basic method to obtain elastic/plastic properties
  - ✓ **Risk point :** Change in the properties w.r.t. the specimen size
    (e.g. test coupon vs. actual probe)
    Supplementary method : Micro tensile test

- **Micro indentation test**
  - ✓ A method to obtain a variety of mechanical properties in a localized region
  - ✓ **Risk point :** Change in the properties w.r.t. indentation depth
    (due to the effects of surface and/or substrate)

- **Micro Compression test**
  - ✓ **Method to make up for micro-indentation test**
  - ✓ **Risk point : Difficulty in predicting the tensile data**


- **Above three methods are used interchangeably and complementally**

# Limitation of the conventional measurement methods

- **A number of tedious iterations during the development of new materials**
  - ✓ High cost and time-consuming process

Make the

for MEMS

# Necessary conditions to evaluate new materials

1. A much faster method

2. A much more affordable method

3. A method to determine the direction of development

# Prediction of the properties using simulation methodology

- **Need to determine the direction of new materials development**
  - ✓ Sometimes very hard to make all the candidates with real substances

**Experimental evaluation for material properties** → **Simulation for material properties**

# Steps for the prediction of properties via molecular dynamics

- **Concept to simulate the properties of a chosen alloy**

Structure/defects with random distribution → Density Functional Theory (DFT) → Molecular Dynamics(MD)

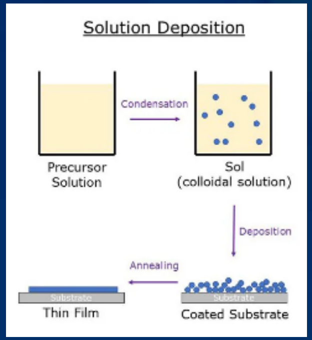
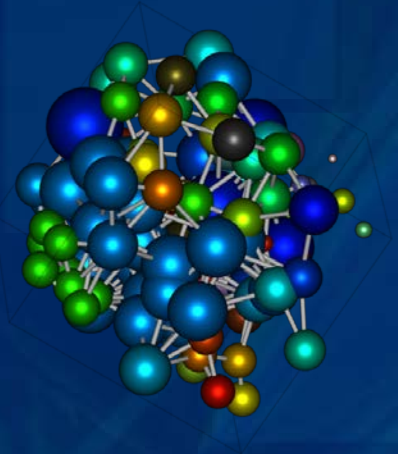
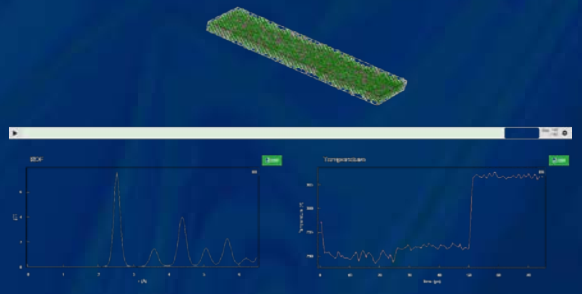



Image source : Sigmaaldrich





- ✓ **Basic Assumption of candidates alloys**
- ✓ **Selection of an alloy**
- ✓ **Verification of properties for a selected alloy**

# Step I : Data acquisition from existing known alloys

- First step to predict the properties of alloy (used in MEMS probes)

Structure/defects with random distribution

Data Acquisition

Data Processing

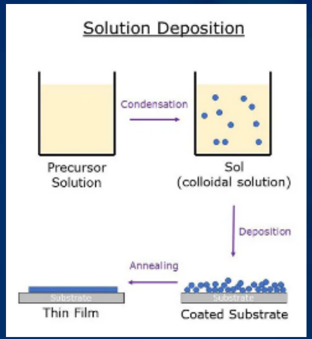
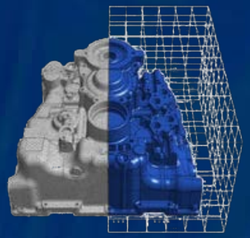



Image source : Sigmaaldrich

In our study, real data was used as the first step



✓ **Basic Assumption of candidates alloys**

✓ **EBSD**

✓ **TEM**

✓ **Mesh free method**

✓ **Confirmed with FEM**

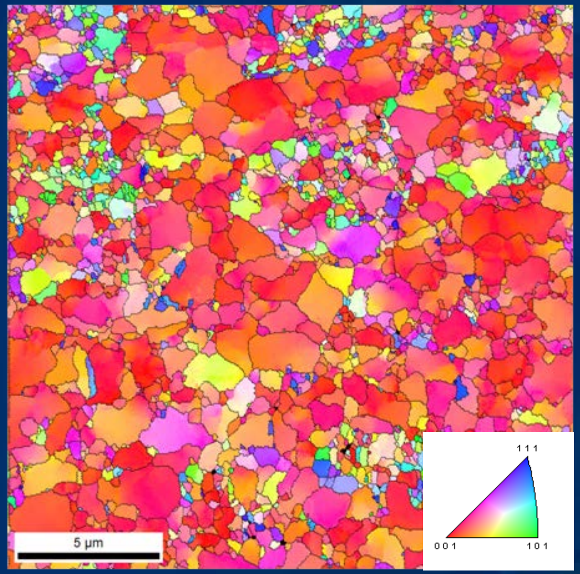
# Data processing by Mesh-free method (MFM)

- **MFM is suitable for crystal-defect sensitive objective with a complex geometry (such as MEMS probes)**

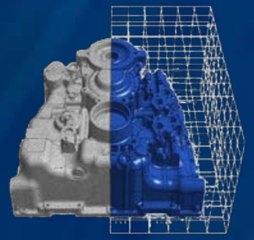
Data Acquisition

Data Processing

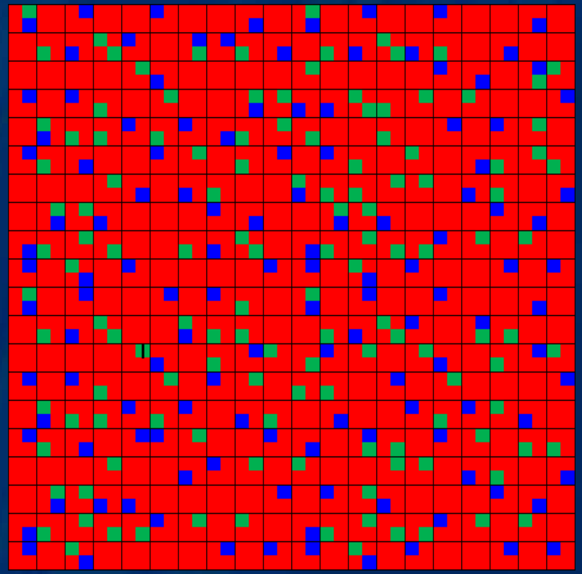
✓ **EBSD**




Sample (About 100 ea)

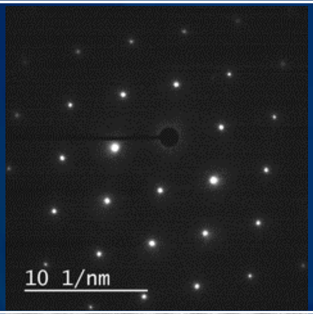
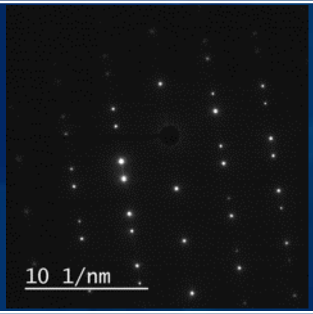
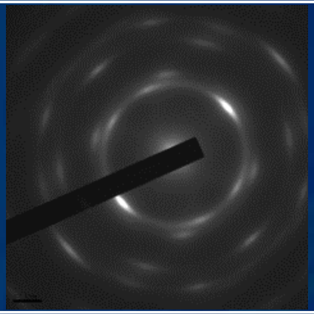
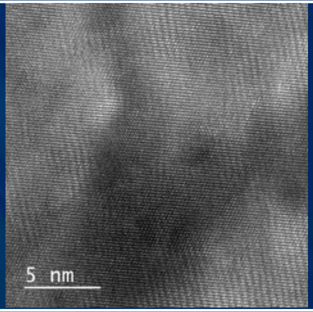
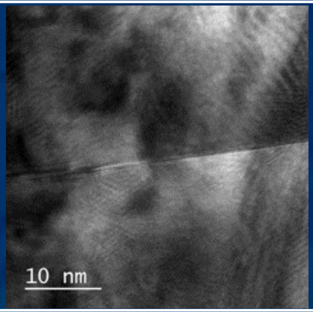
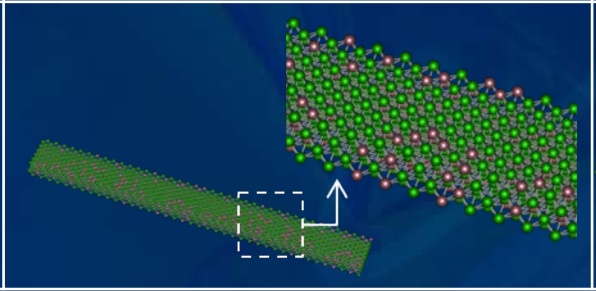
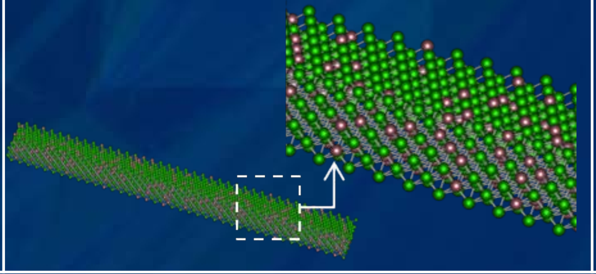
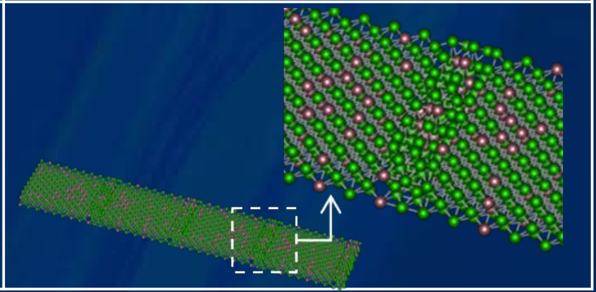


✓ **MFM**



# Step II: DFT-based structural modeling

- **DFT modeling is able to accommodate a variety of crystal structures/defects**

| | Single Crystal (SC) | Twin | Poly Crystal (PC) |
|---|---|---|---|
| SAED Pattern |   |   |  |
| HR-TEM |   |   |  |
| Structural modeling |  |  |  |

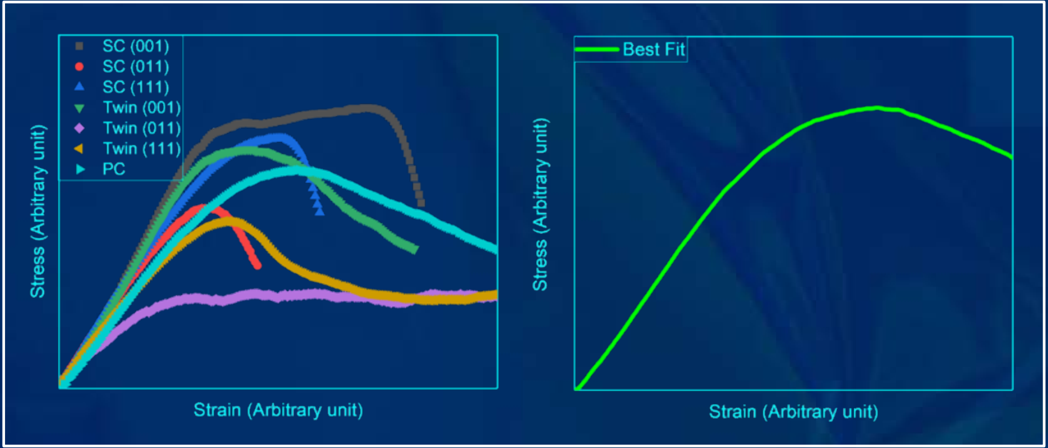
# Step III : MD simulation and fitting

- **Performing stress-strain(S-S) simulations using MFM and MD**

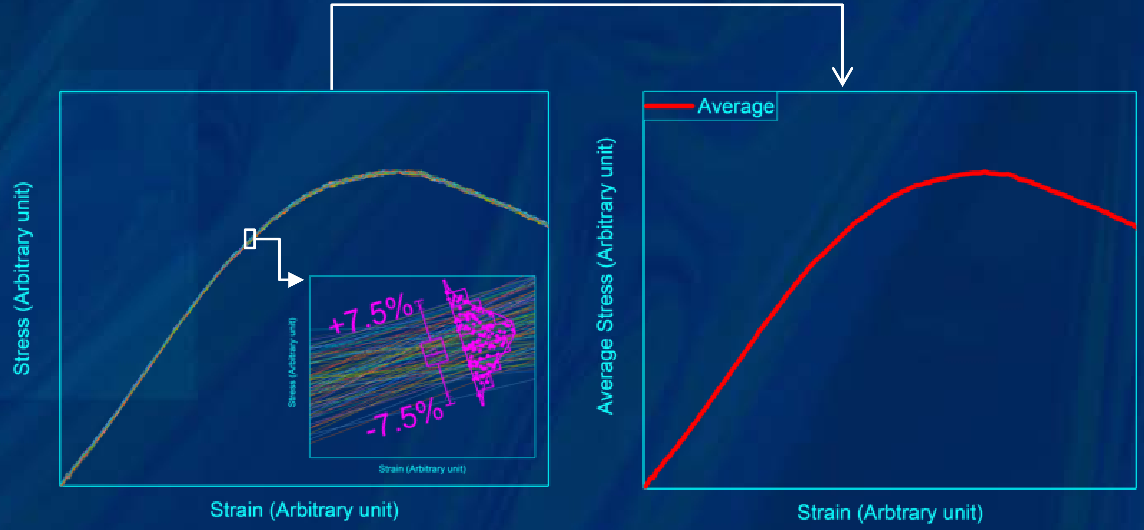
$$S\text{-}S_{simulation} = Normalized\ Factor \times [\ (\alpha \times SC\ S\text{-}S_{simulation}) + (\beta \times PC\ S\text{-}S_{simulation}) + (\gamma \times Twin\ S\text{-}S_{simulation}) + \delta(Crystal\ defects)\ ]$$

Data Processing → DFT → MD → Statistical analysis → Trend Curve Fitting

Repeat x 100 times
(A hundred samples)




x 100 times

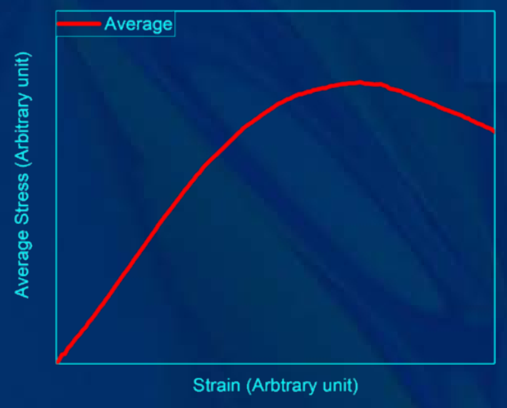


# Validation of MD Simulation with a real probe

# Validation of MD Simulation with a real probe

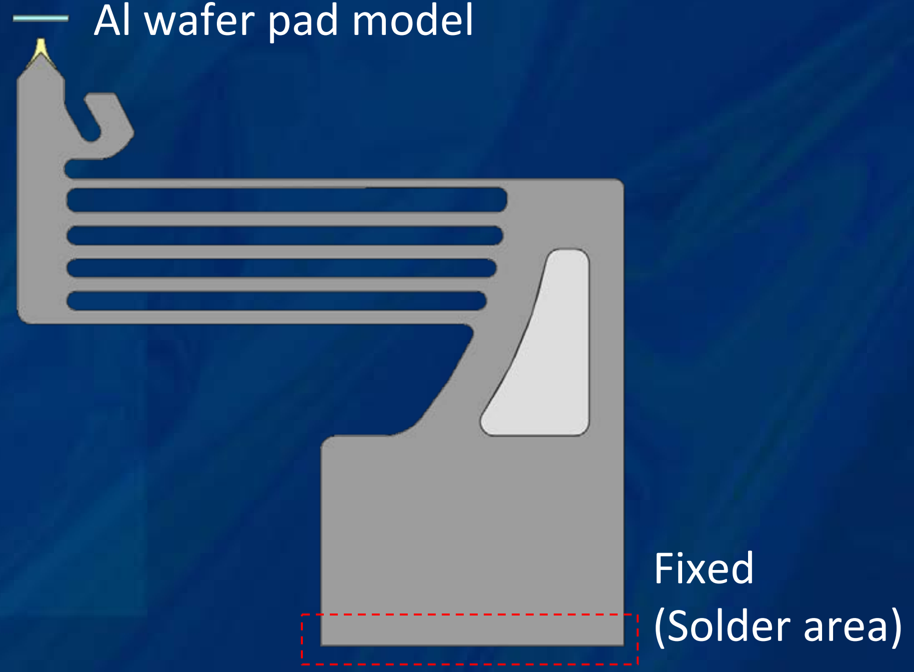
- **Start the simulation using the data from trend curve fitting**

Trend Curve Fitting




✓ Stress-Strain data from MD Simulation

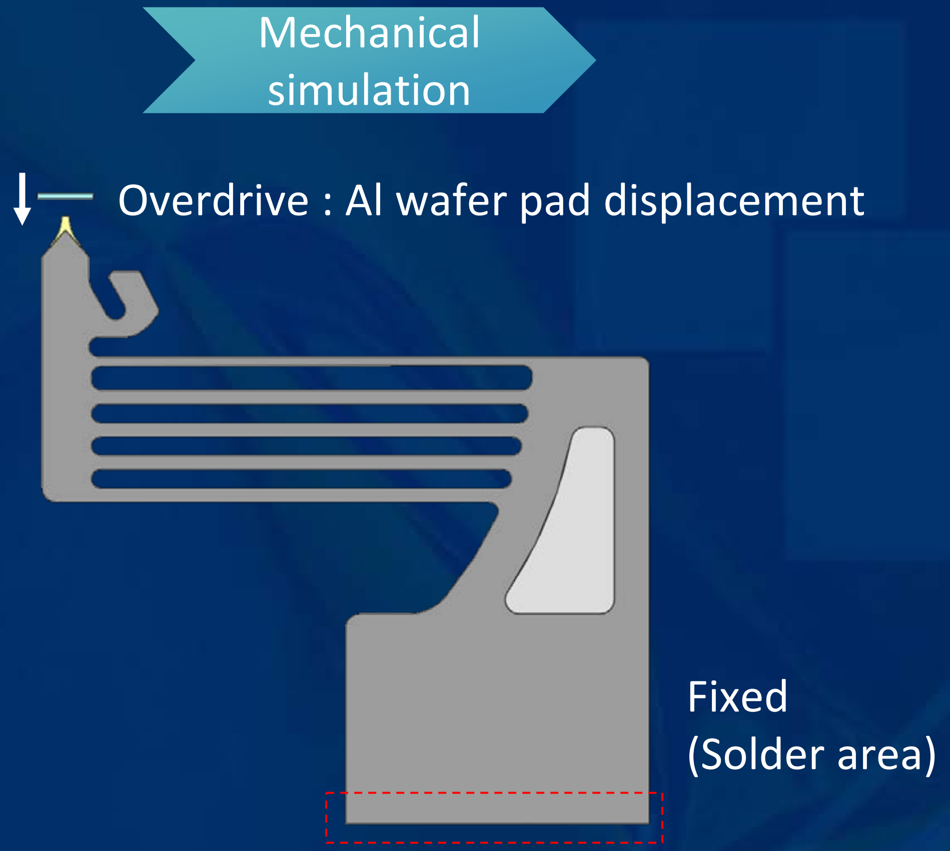
Mechanical simulation




✓ Typical probe shape (Not an actual product)

# Cognitive Simulation of MEMS Probe - Mechanical Aspect

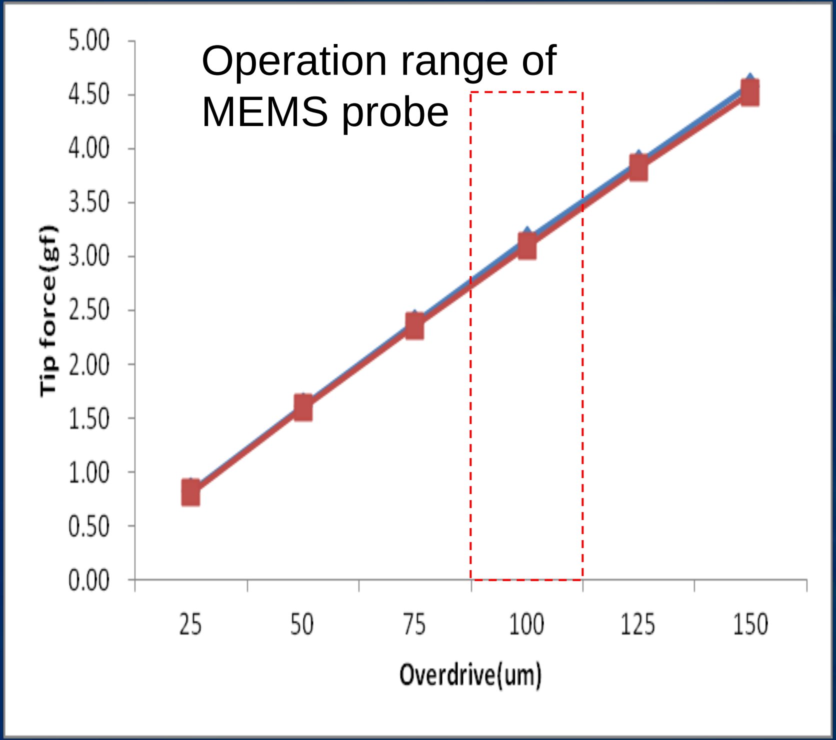
- **Preparation of simulation conditions and the necessary data set**

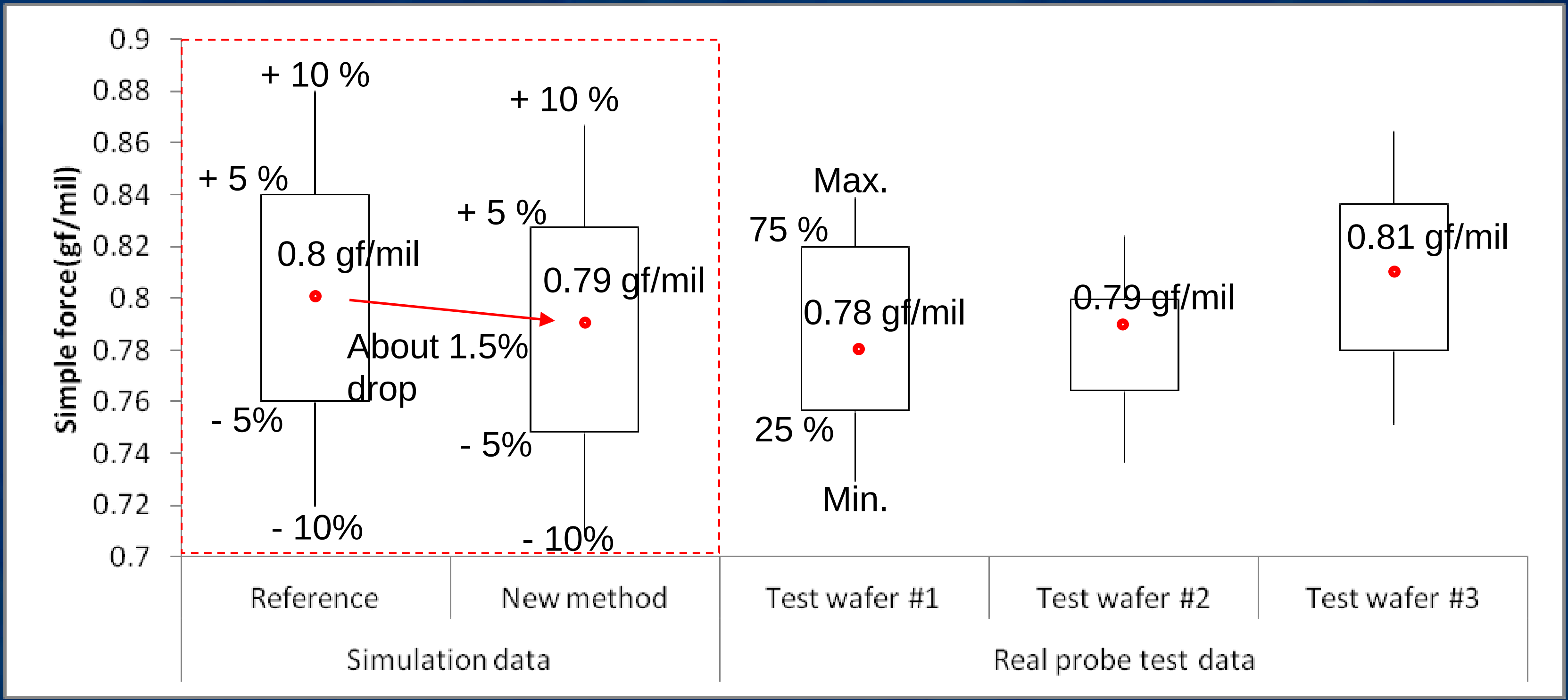



- **Mechanical simulation for tip force**
  - ✓ Non-linear simulation
  - ✓ Implicit method, dynamic method
  - ✓ Quasi-static analysis
  - ✓ Fixed : Solder area
  - ✓ Overdrive(Load) : Displacement
- **Al pad property for simulation**
  - ✓ Modulus : 68 GPa
  - ✓ Poisson's ratio : 0.36
  - ✓ Yield stress : 105 MPa
  - ✓ Density : 2.70 g/cm$^3$
  - ✓ Second hardening modulus : 680 MPa

# Cognitive Simulation of MEMS Probe - Mechanical Data

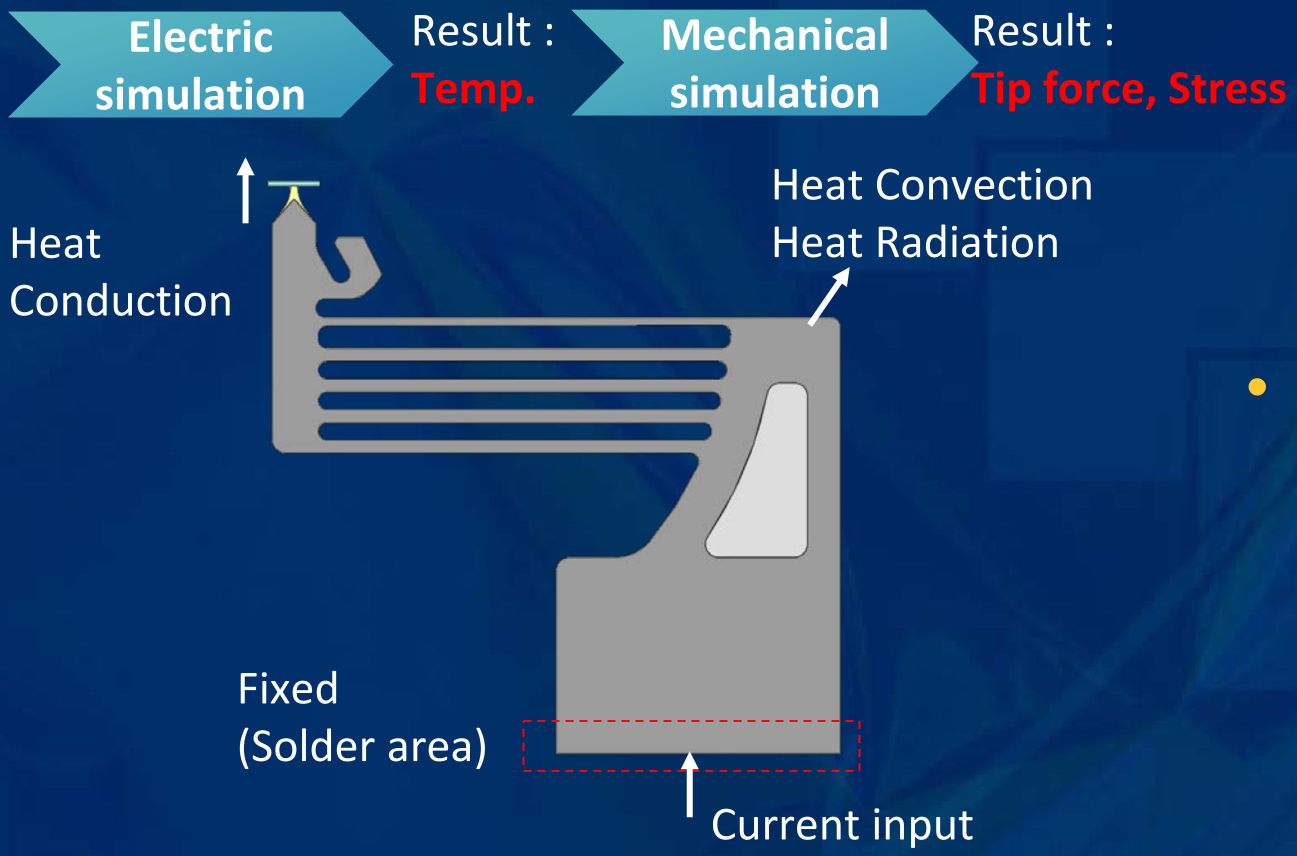
- **Prediction of Tip Force (spring const.) Results**
  - ✓ The difference between the simulation and measurement data is approximately 1.5%.
  - ✓ This is well within the manufacturing tolerance of MEMS probes.
  - ✓ The predicted properties using our method shows a high consistency.



# Cognitive Simulation of MEMS Probe - Electrical Aspect

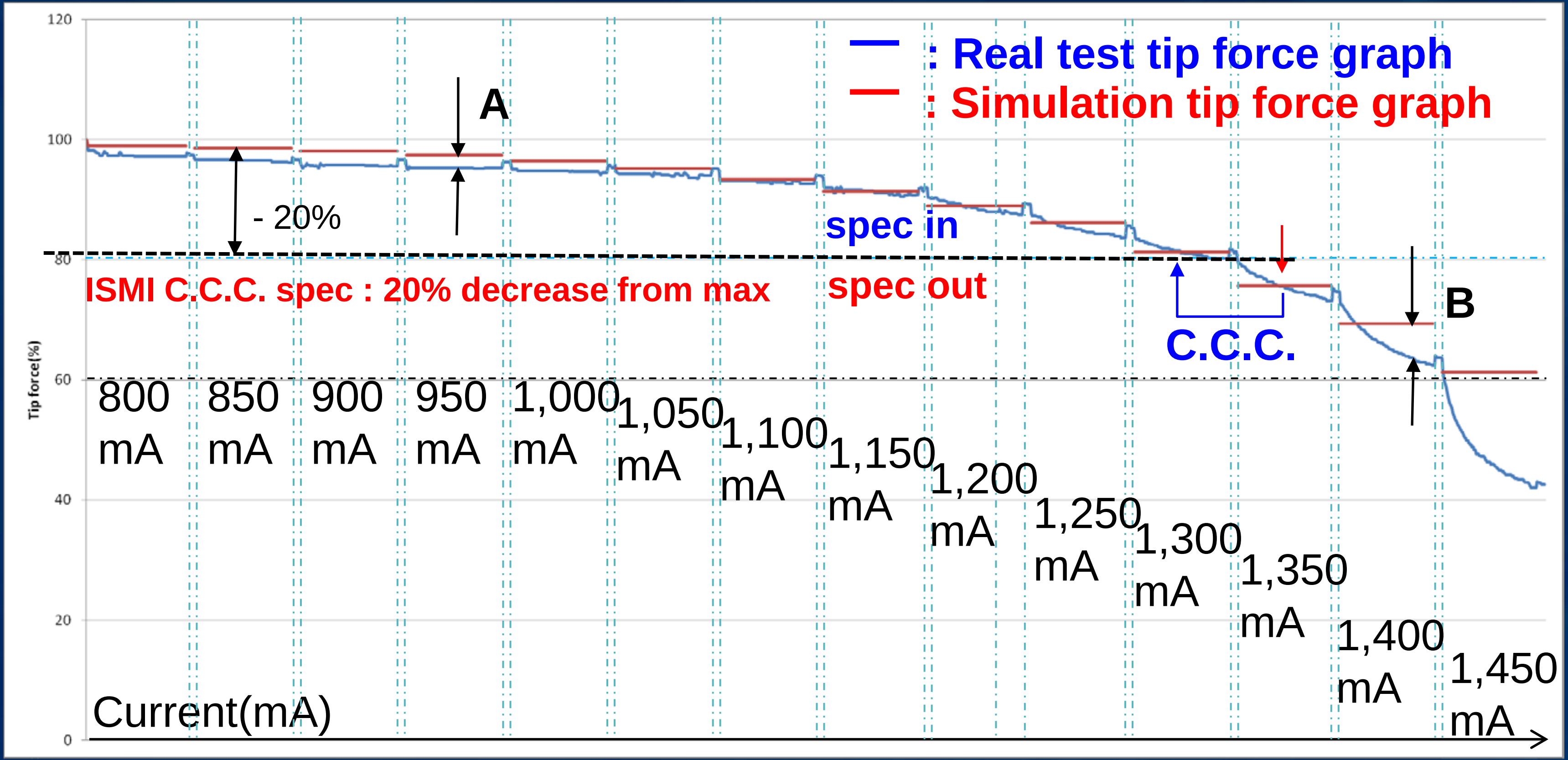
- **C.C.C.(current carrying capability) is the most important electrical property.**
  **- C.C.C. is highly dependent on the mechanical and thermal properties.**

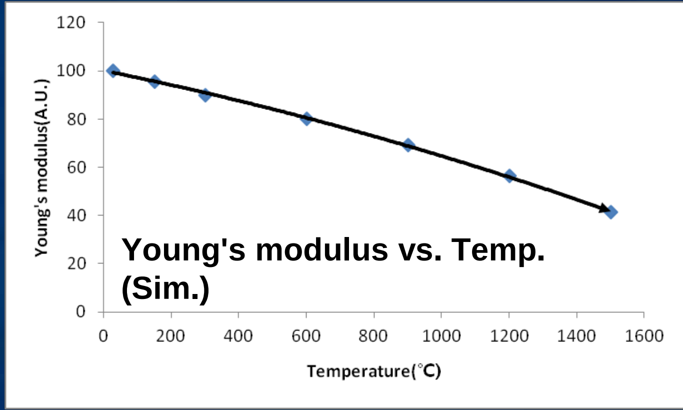


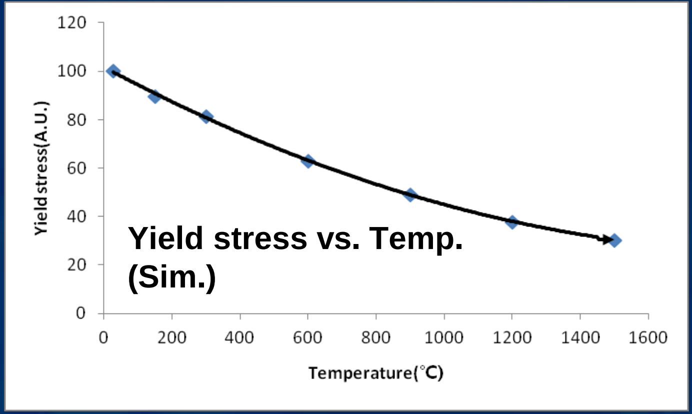

- **Electric simulation (for C.C.C.)**
  - ✓ Joule heating simulation
  - ✓ Contact resistance : Constant
  - ✓ Conduction coefficient : Constant
  - ✓ Convection coefficient : Constant
  - ✓ Radiation coefficient : Constant
- **Al pad property for simulation**
  - ✓ Non-linear simulation
  - ✓ Implicit method, dynamic method
  - ✓ Quasi-static analysis
  - ✓ Fixed : Solder area
  - ✓ Overdrive(Load) : Displacement

# Cognitive Simulation of MEMS Probe - Electrical Data

- **Force drop w.r.t. current : measured data > simulated data**
  - ✓ Decreases in Young's modulus and Yield strength lead to tip force decrease.
    - Middle current region (800 -1250 mA) : relatively small gap denoted by "A"
    - High current region (> 1250 mA) : considerable gap denoted by "B"

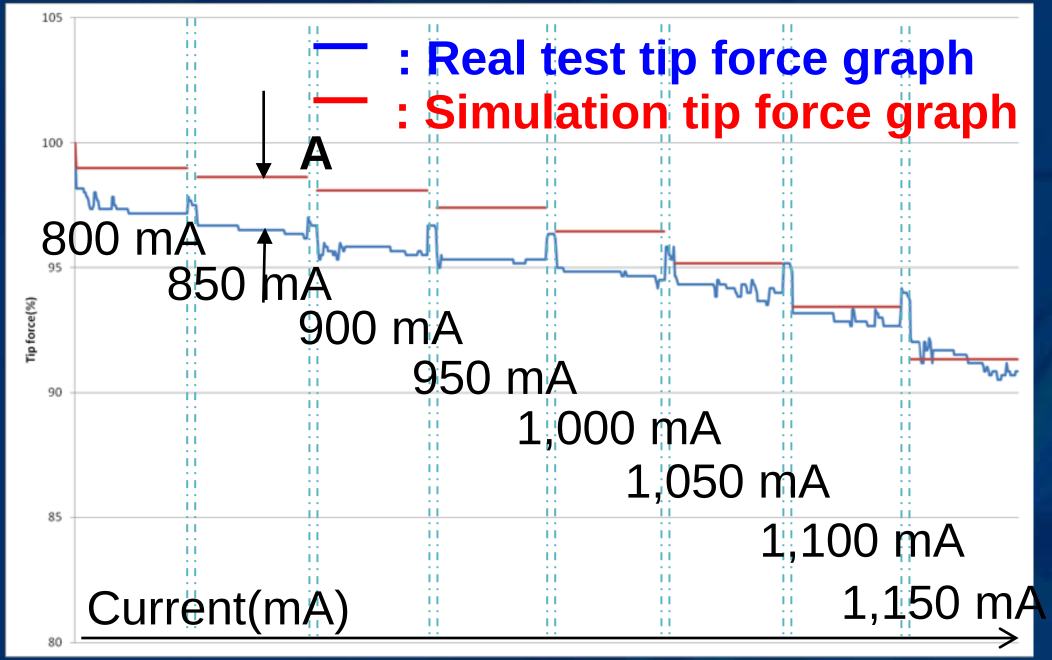


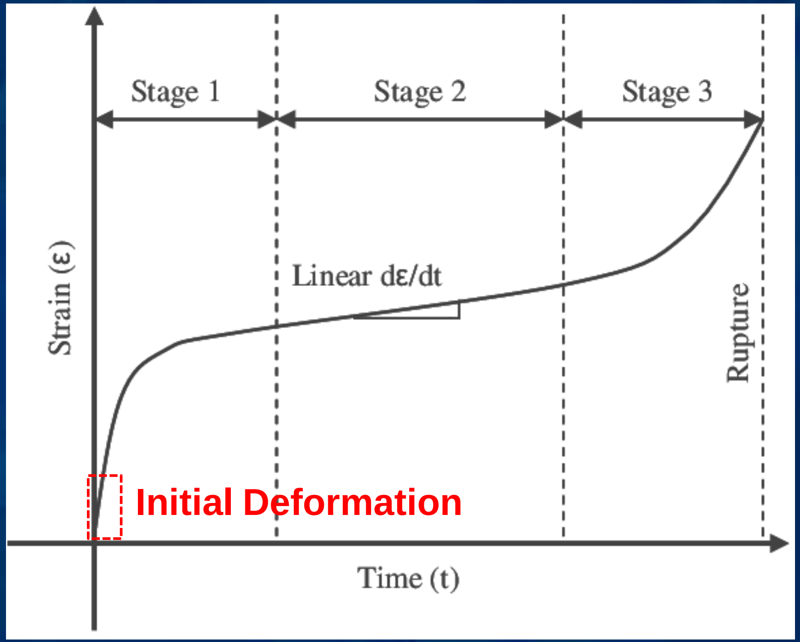



# Cognitive Simulation of MEMS Probe - Gap analysis A

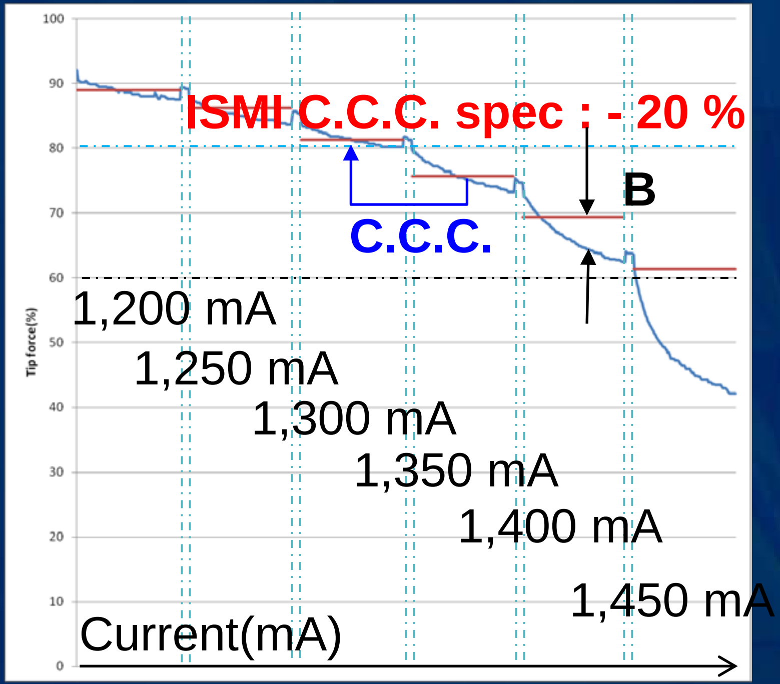
- **Small gap (up to 1,150mA) between measured and simulated data (A)**
  - ✓ Relatively large deformation at the very beginning of test
  - ✓ Hard to quantitatively predict due to the extrinsic factors (heat treatment etc.)

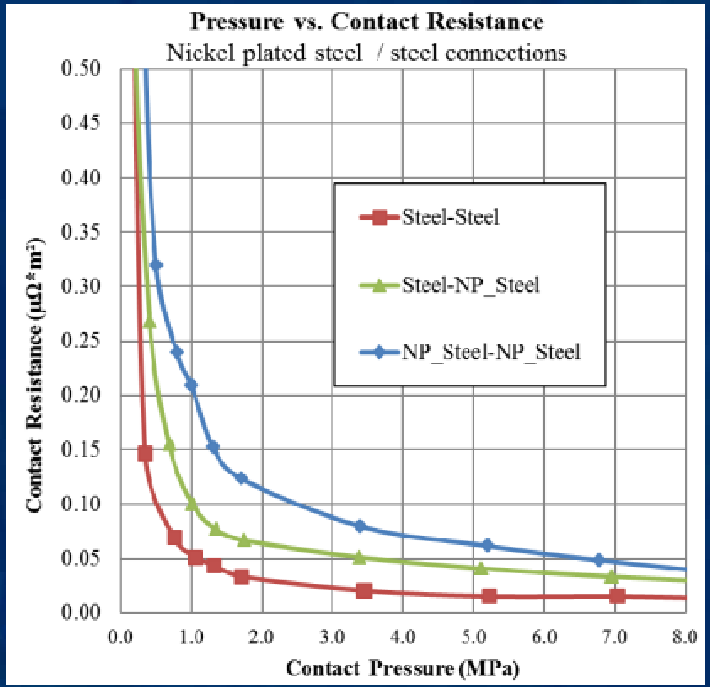


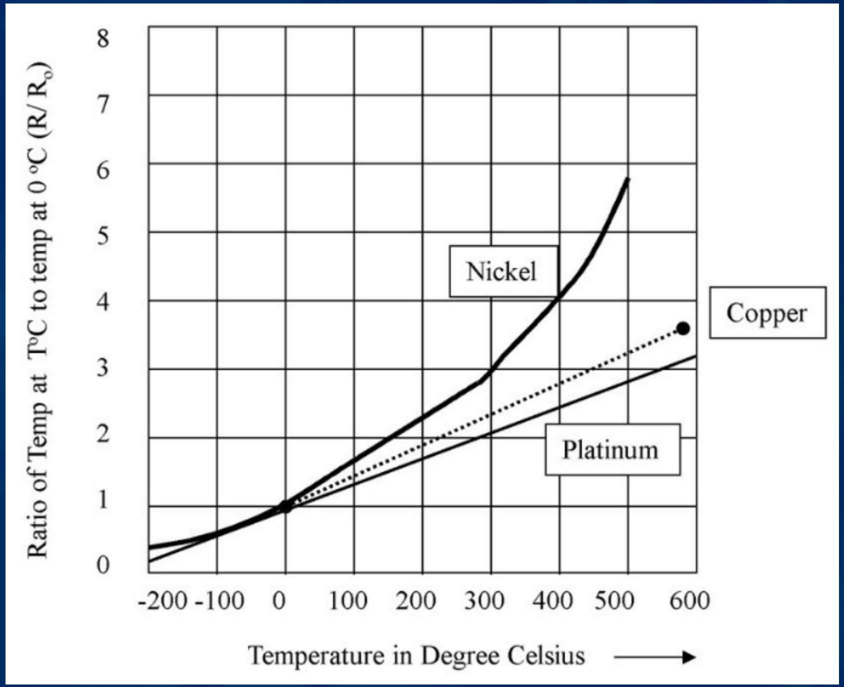
# Cognitive Simulation of MEMS Probe - Gap analysis B

- Large gap (>1,150mA) between measured and simulated data (B)
  - ✓ High Current → Joule heating → Decrease in Young modulus → Contact R increase
    repeat
  - ✓ Metals show different behaviors of R-increase with temperature




" Contact Resistance versus Pressure of Electrical Connections Used in Aluminium Smelter Potlines ", W.Berends




" Research and Design of Snow Hydrology Sensors and Instrumentation " , Raman K. Attri

# Summary

- We suggested the simulation methodology to predict and validate the properties of new materials for MEMS probe application.
  - ✓ To predict the mechanical properties of new materials, Molecular Dynamic (MD) based tool was mainly used.
  - ✓ Prior to MD simulation, we performed data processing on crystal defect/structure and simulation based on Density Function Theory (DFT).

- To verify the consistency of our simulation methodology, we simulated the mechanical properties for a known material.
  - ✓ Key mechanical properties of real probe (tip force vs. current) were predicted in comparison with measured values.
  - ✓ Although the overall trend is similar, the gap existed such that it became larger in higher current region.
  - ✓ The gap is due to initial deformation and contact resistance characteristics, where some of the materials properties can be obtained by measurement only at this point.

# Future works

- Additional information for the completeness of MD Simulation
  - ✓ Material creep behavior at the very beginning stage

- Additional simulation areas that can replace experimental methods
  - ✓ Dependence of contact resistance on tip force and contact area
  - ✓ Further study on contact resistance, related to

    -. Fretting phenomenon caused by mechanical movement and/or thermal expansion

    -. Self-cleaning effect that typically helps to decrease the resistance
  - ✓ Fritting, a melting/softening phenomenon, occurring when the voltage reaches a critical point.

If you have any questions,

PLEASE SEND an e-mail

(E-mail address : teakongjuni@kicl.co.kr)