Constitutive modelling of silicon under nano-scale deformation

Tania Vodenitcharova and Liangchi Zhang

School of Aerospace, Mechanical and Mechatronic Engineering

The University of Sydney

Current project on Silicon

Aim of project:

develop a constitutive model for phase transformation of Si

Why a new project?

existing models cannot be applied

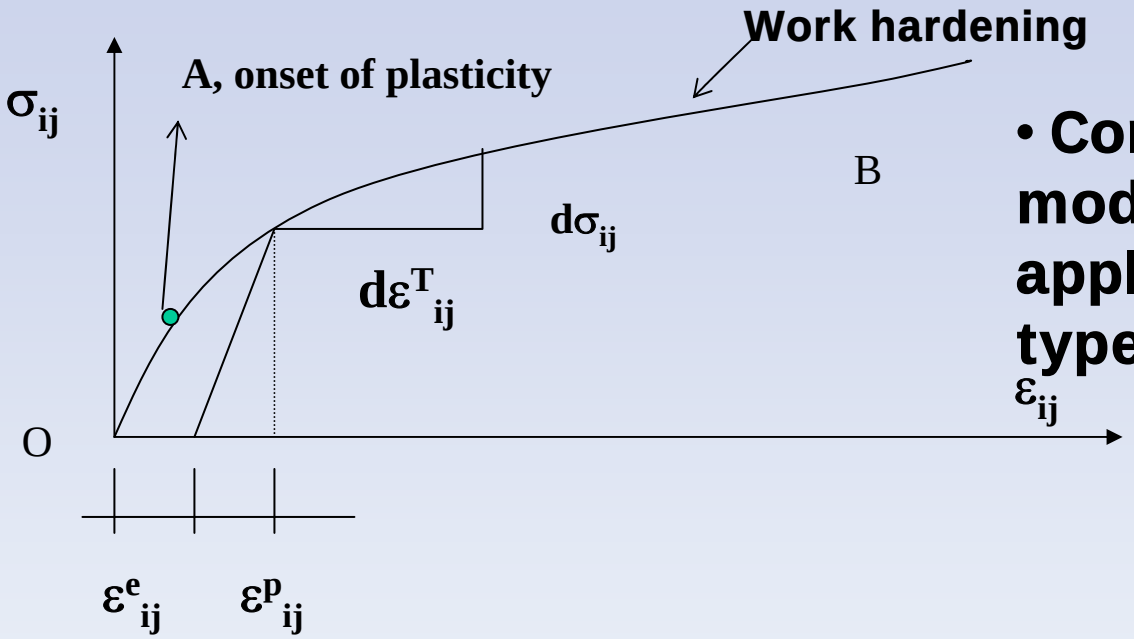
What is a constitutive model?

mathematical formulation of physical behaviour of materials

What does constitutive model consist of?

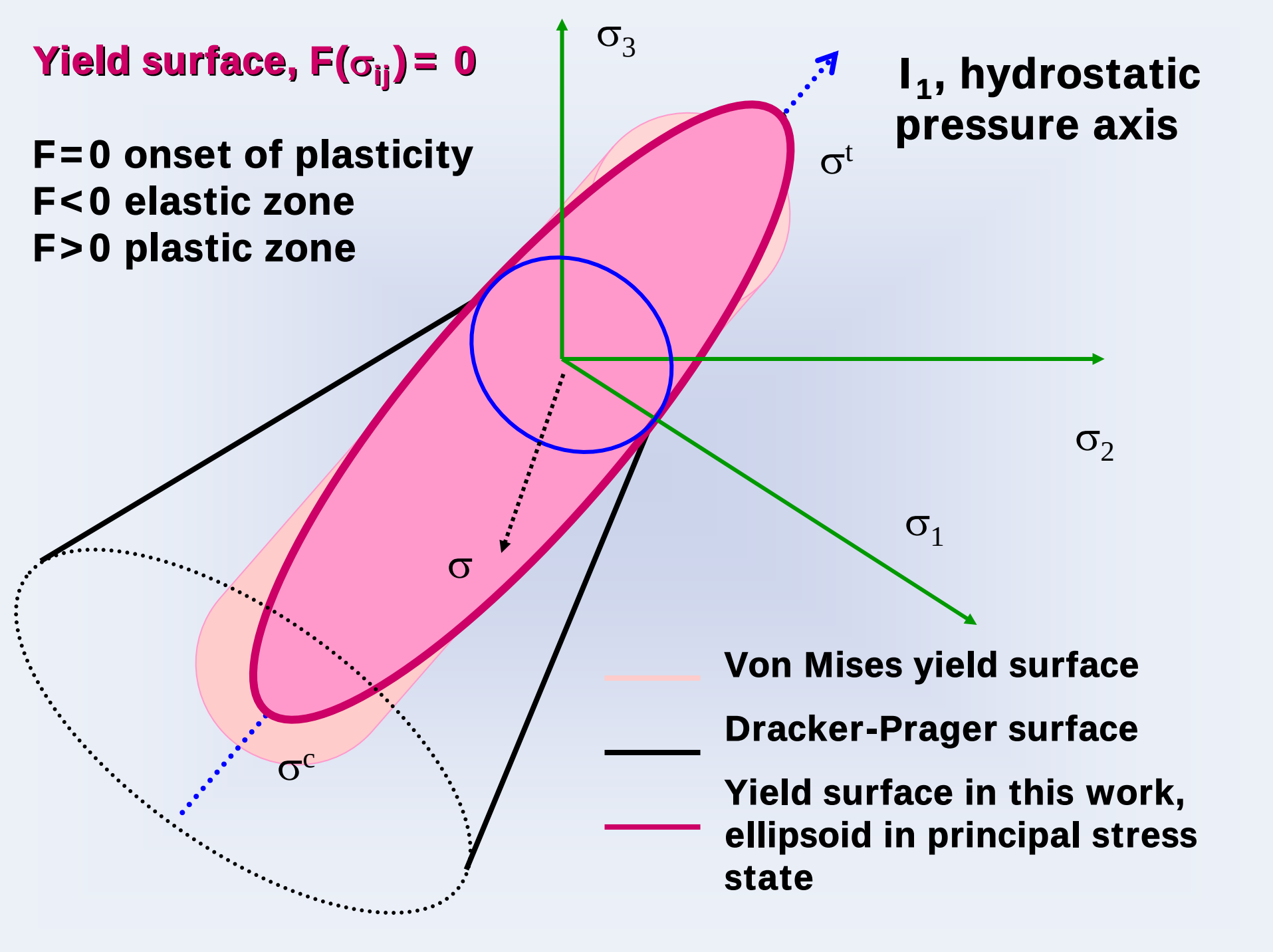
- **prediction of onset of plasticity- due to phase change**
- **developing of stress/strain relationship**

Stress/strain relationship



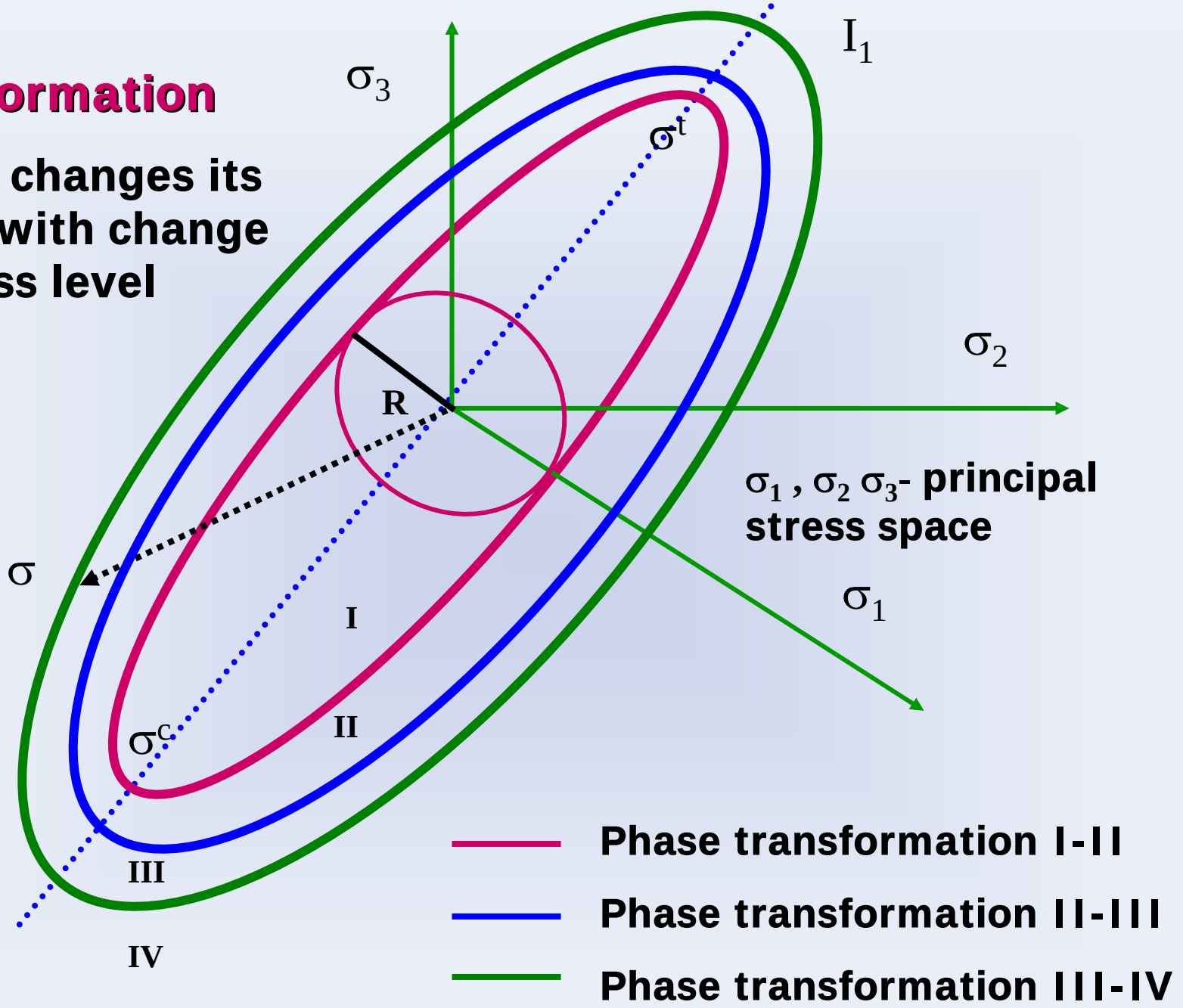
- **Constitutive model is applicable to any type of load**

OA- elastic, AB elastic-plastic, $\varepsilon^T_{ij} = \varepsilon^e_{ij} + \varepsilon^p_{ij}$, $d\varepsilon_{ij}{}^p = d\varepsilon_{ij}{}^{p,\,deviatoric} + d\varepsilon_{ij}{}^{p,\,volumetric}$


Yield surface, F(σij)= 0
F=0 onset of plasticity
F<0 elastic zone
F>0 plastic zone
σ3
σt
I1, hydrostatic pressure axis
σ2
σ1
σ
σc
Von Mises yield surface
Dracker-Prager surface
Yield surface in this work, ellipsoid in principal stress state

Phase transformation

Silicon changes its phase with change in stress level



What do we need to develop?

Incremental stress-strain relation:

$\{d\sigma\} = [C(\sigma_{mn})]\ \{d\varepsilon\}$, [C]- constitutive matrix is derived

Yield function:

$F(\sigma, \varepsilon) = (\sigma^{eff})^2 + 1.5\ R^2\ I_1^2 / [\sigma_m - (\sigma^t + \sigma^c)/2]^2 - 1.5R^2 = 0$

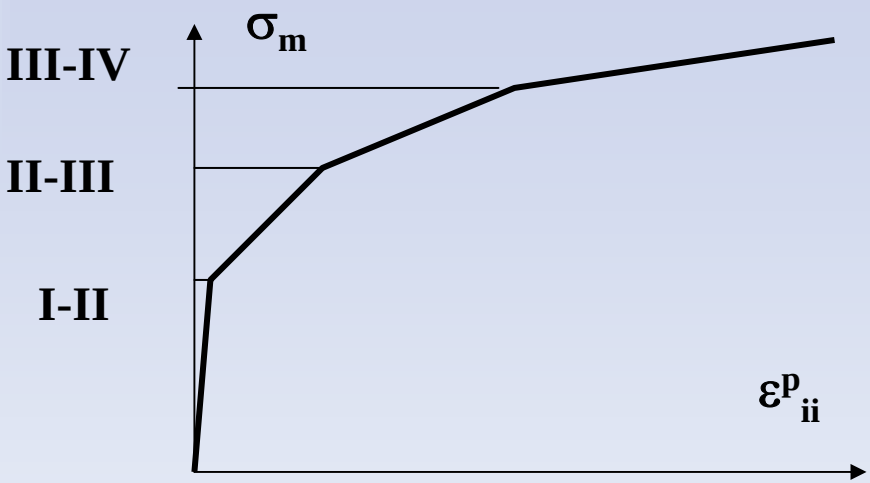
material constants: E, K; σ^t ,σ^c , R for each phase

$F < 0$ elastic, $F > 0$ plastic

Flow rule:

$d\varepsilon_{ij}^p = \lambda\ \partial F / \partial \sigma_{ij}$, associated normality, isotropic hardening

Hardening is prescribed by hydrostatic pressure tests



- Assumed **multi-linear**
- Given by hydrostatic pressure tests/ molecular dynamics simulations
- Yield surface **uniformly expands** along the semi-axes of ellipsoid

FEA Simulations