Integrated Computational Materials Engineering: Recent Progress in the Advanced Titanium Microstructure and Modeling Program

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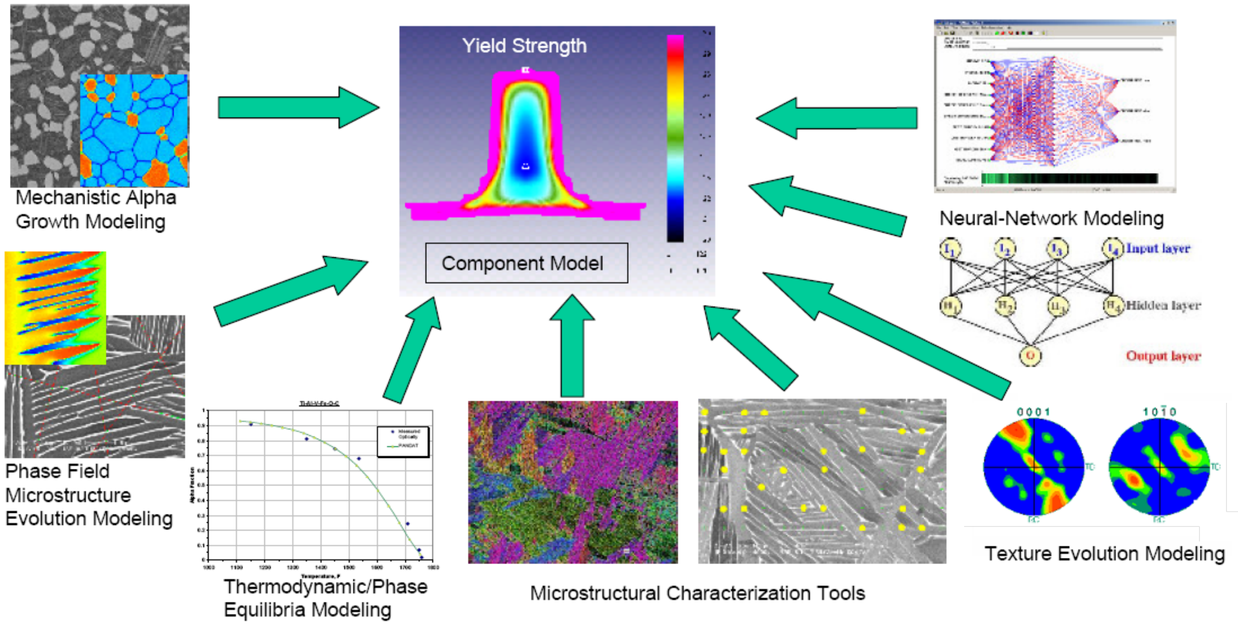
Review of previous MAI program results - Ti modeling 1 (LAD-2)

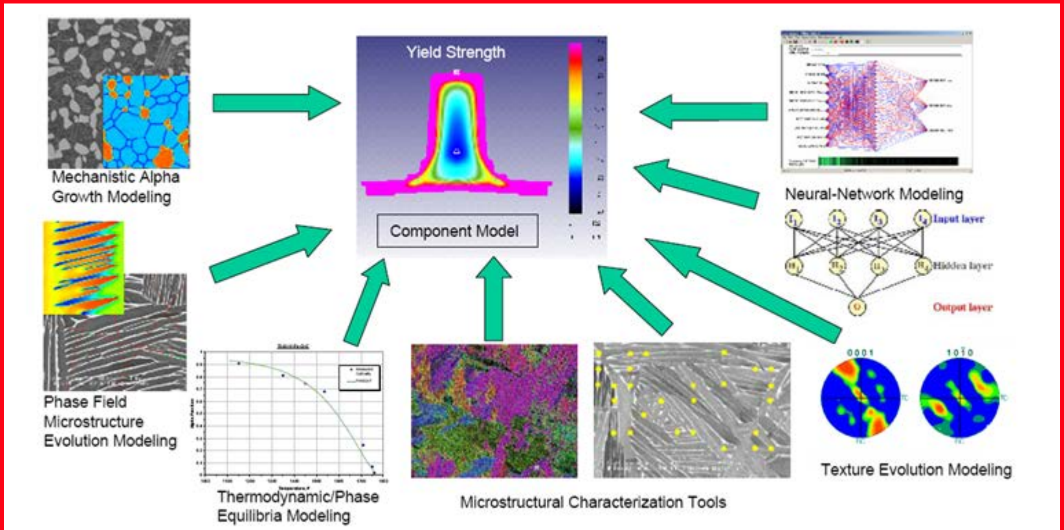


Program summary

- Modeling tools that predict microstructure evolution were successfully developed and demonstrated for **beta processed and alpha-beta processed** Ti-6Al-4V
- Mechanical property models were successfully developed and demonstrated on full-scale production components
- A neural net that linked microstructure quantities and chemistry to mechanical properties (YS, UTS, %El, RA,KQ, K1C) was developed

Review of previous MAI program results - Ti modeling 2 (LAD-4)

DEFORM

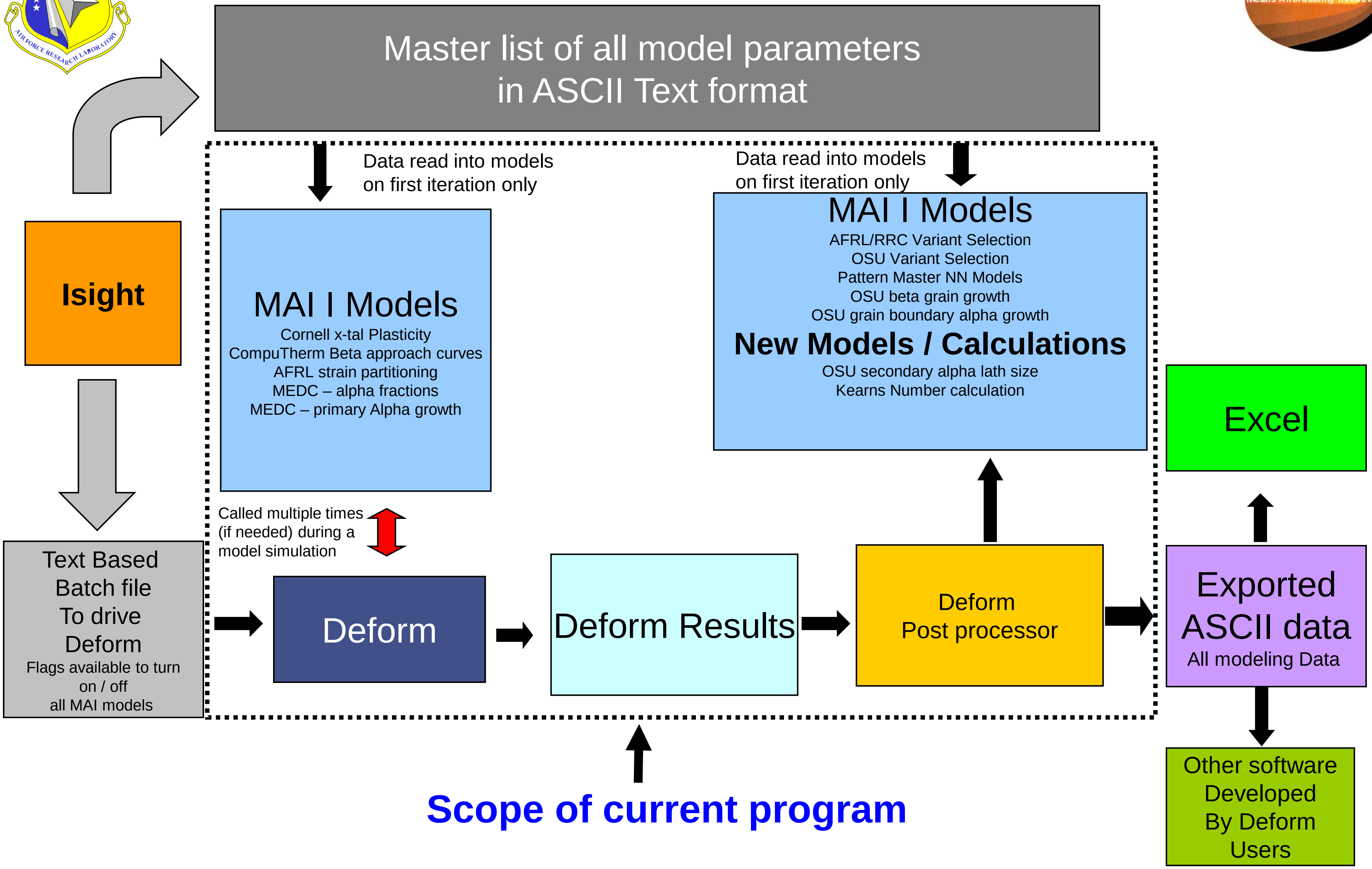


Program summary

- Established the feasibility of integrating Ti Modeling 1 tools into maintainable, user friendly FEM software tools such as DEFORM
- Established the feasibility of extending Ti Modeling 1 models to advanced titanium alloys
- Established the feasibility of developing modeling tools that predict mechanical properties that support component lifing optimization

Rolls-Royce

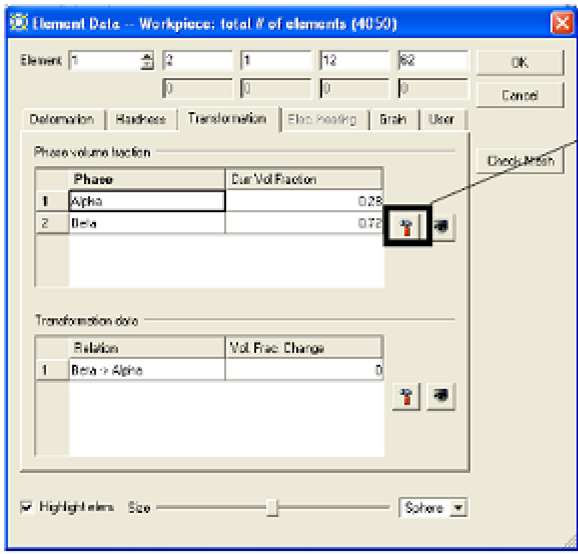
MAI RR-10 Software integration master vision

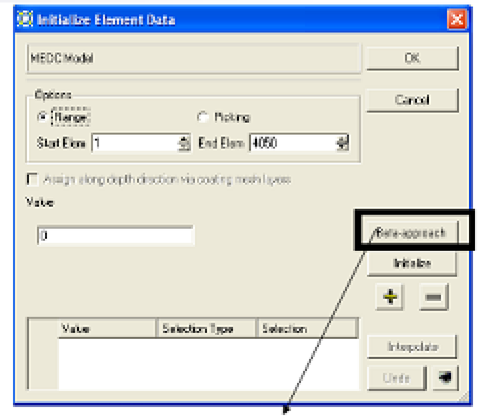


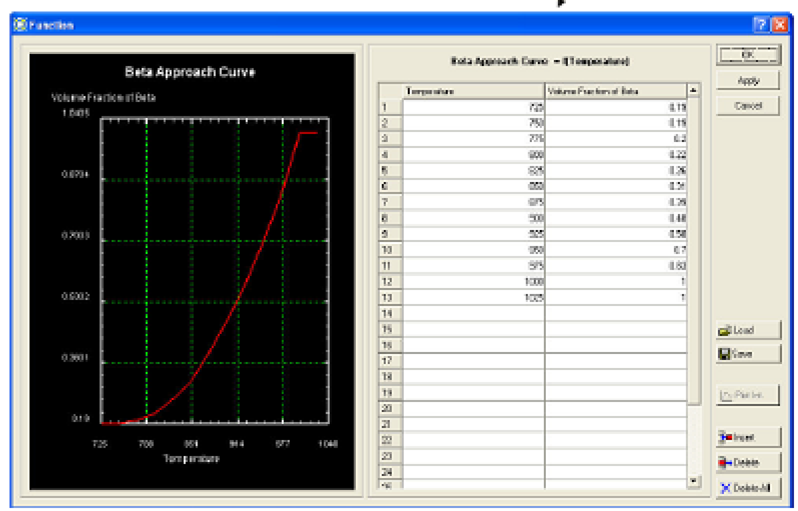
Thermodynamic database integration

Integrate Pandat calculations with DEFORM through look-up tables

- Initialize state variables:
  - Input beta approach curve from CompuTherm







Rolls-Royce

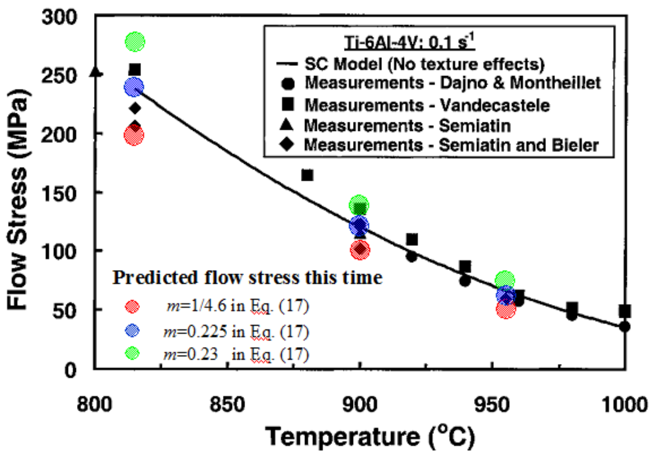
Integration of strain partitioning for Ti-6Al-4V

Self-consistent model

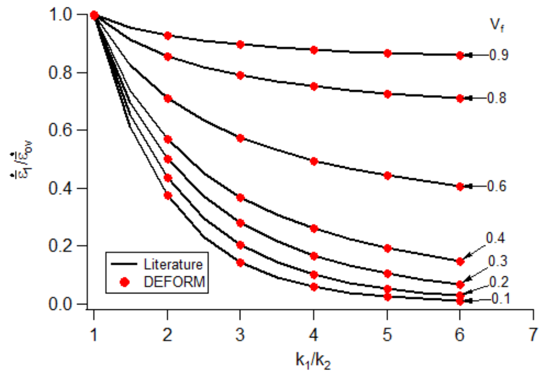
$$\sigma_{ov} = k\dot{\varepsilon}_{ov}^{m} = fk_1\dot{\varepsilon}_1^{m} + (1-f)k_2\dot{\varepsilon}_2^{m}$$

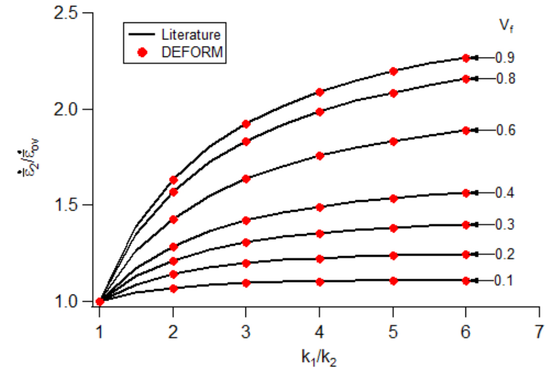
$$\dot{\varepsilon}_{ov} = f\dot{\varepsilon}_1 + (1-f)\dot{\varepsilon}_2$$

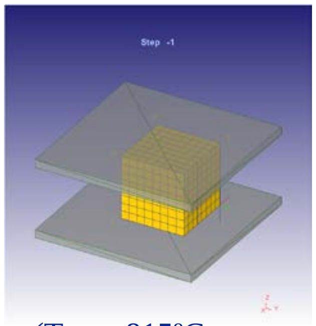
Prediction of flow stress



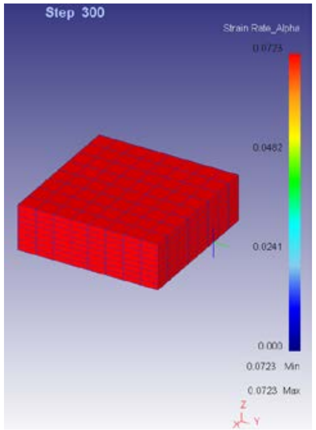
Integration and Validation

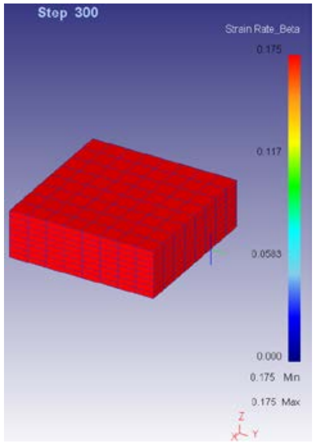






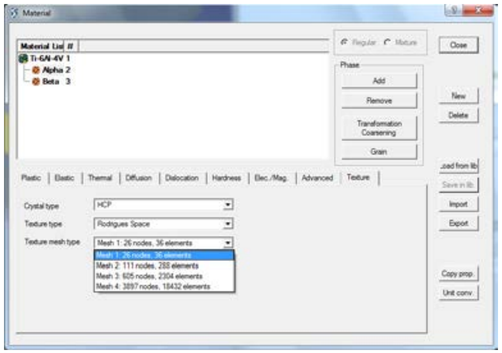
(Temp:815°C; volume fraction: 0.73)

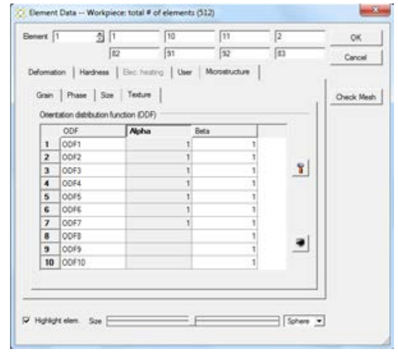


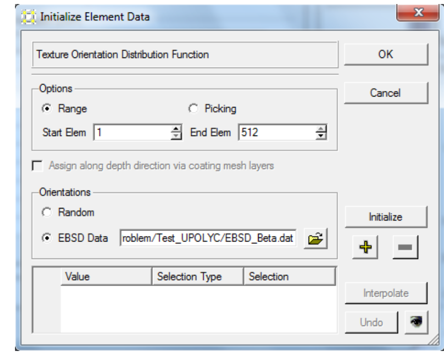


Integration of a crystal plasticity model framework

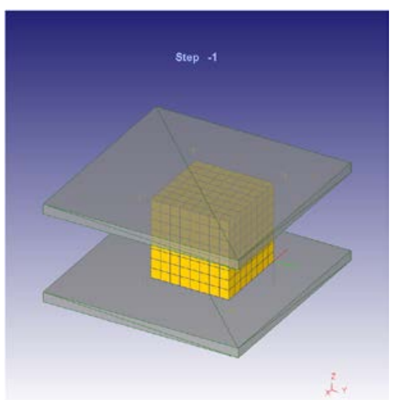
GUIs: texture definition and local initialization



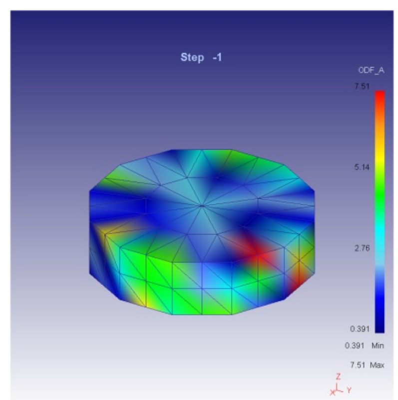




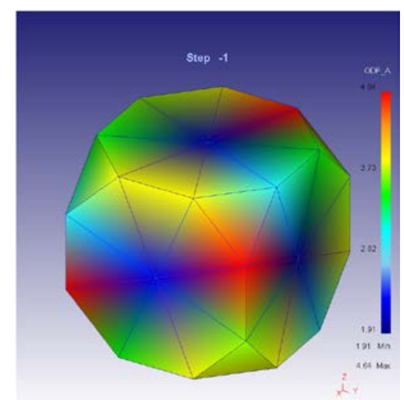
Texture analysis and display



FEA model



Alpha phase

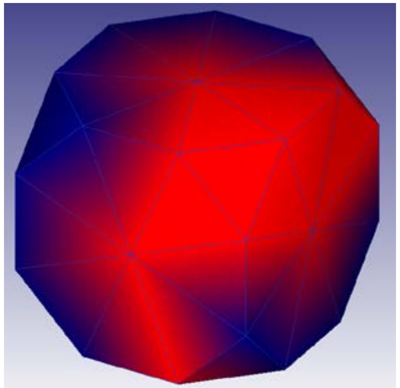


Beta phase

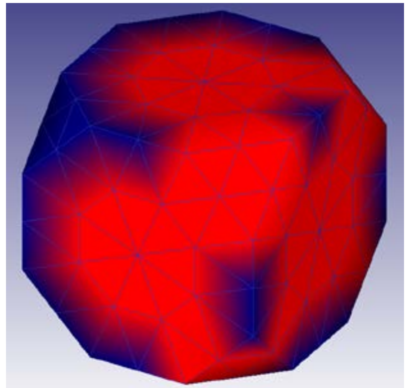
Crystal plasticity model framework

Rodrigues representation of crystallographic texture

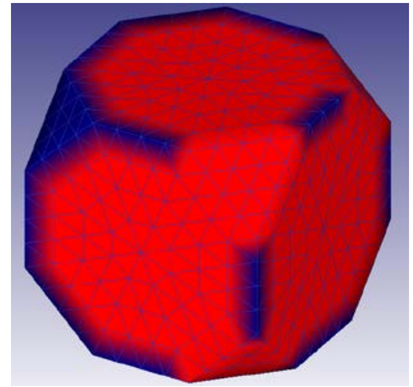
(BCC: Beta phase)



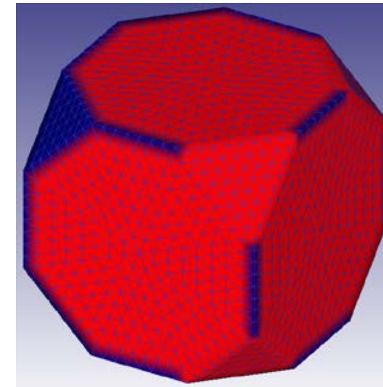
(31 nodes, 56 elements)
(10 independent nodes)



(145 nodes, 448 elements)
(76 independent nodes)

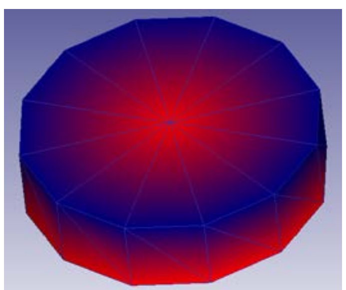


(849 nodes, 3584 elements)
(600 independent nodes)

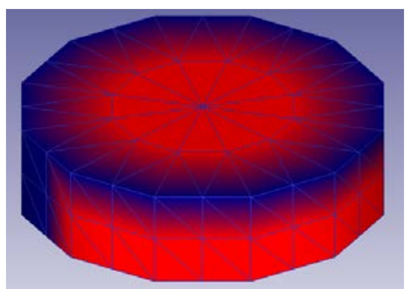


(5729 nodes, 28672 elements)
(4784 independent nodes)

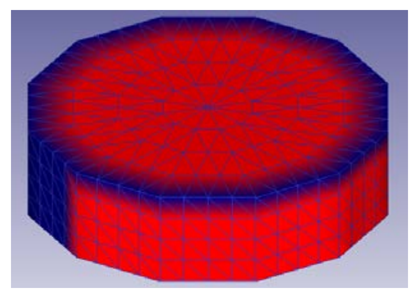
(HCP: Alpha phase)



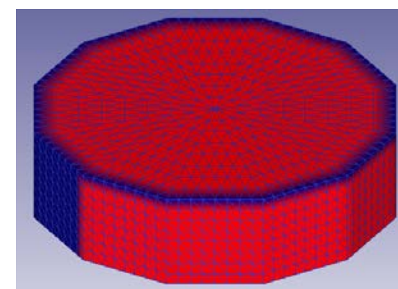
(26 nodes, 36 elements)
(7 independent nodes)



(111 nodes, 288 elements)
(50 independent nodes)



(605 nodes, 2304 elements)
(388 independent nodes)



(3897 nodes, 18432 elements)
(3080 independent nodes)

Least Accurate
Short Run Times

Variable Resolution

Most Accurate
Long Run Times

Primary alpha growth model integration

Integration

Input

Initial volume fraction and particle size
(β approach curve, phase composition, diffusion coefficients)
Cooling rate

↓

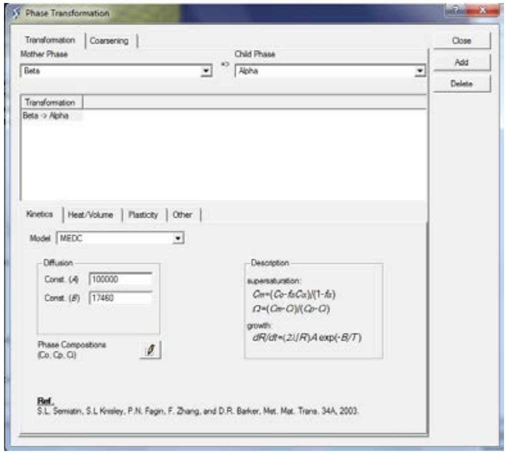
MEDC
GUI + FEM Engine

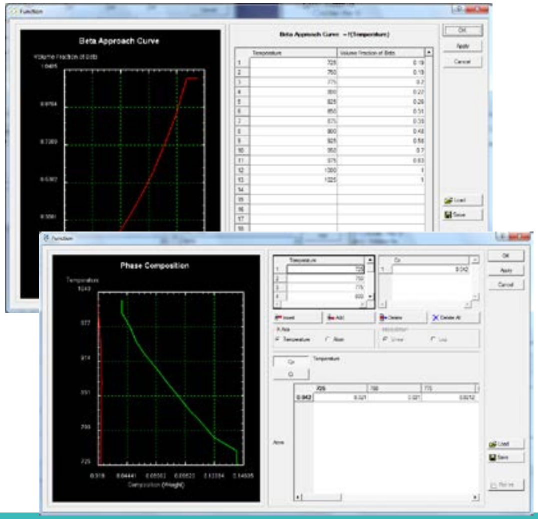
↓

Output

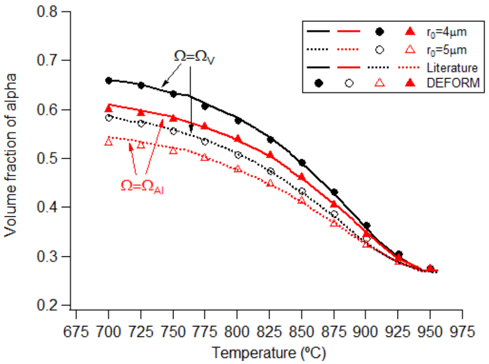
Volume fraction of primary Alpha
And grain size distribution

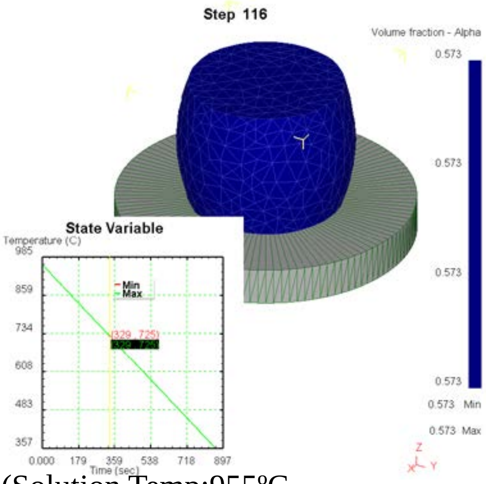
GUIs





Validation

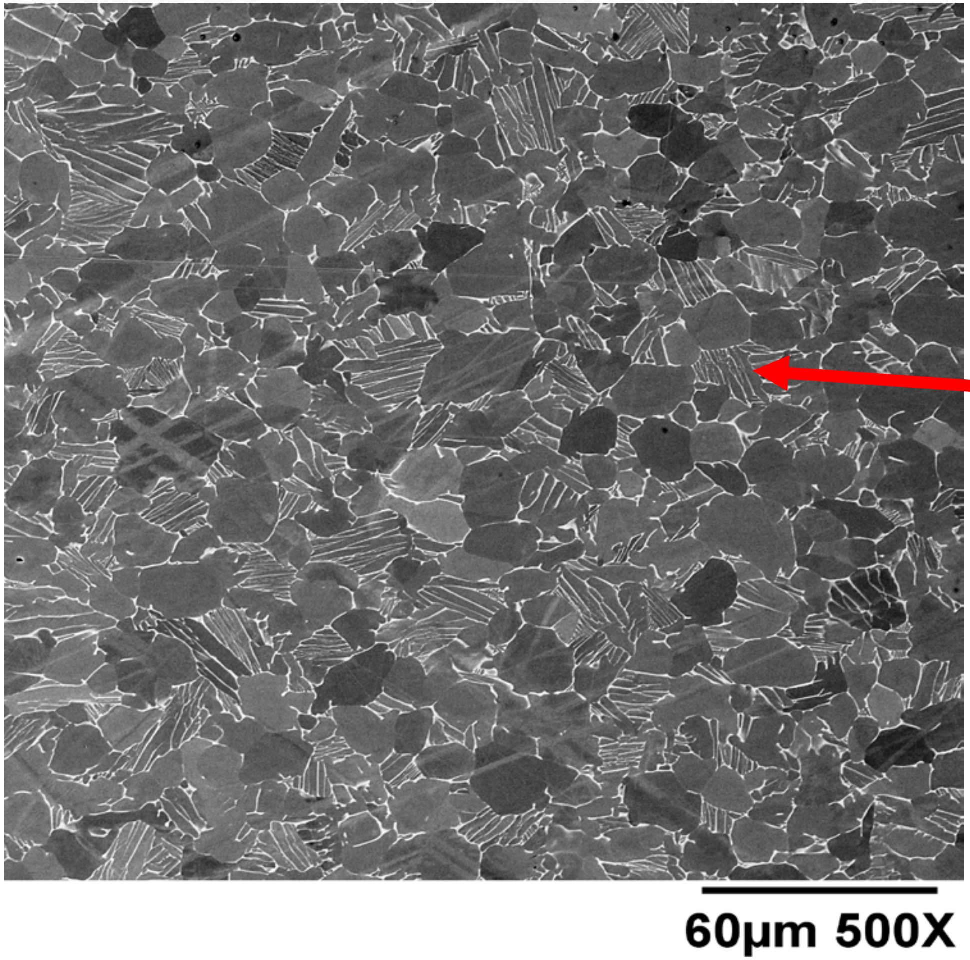




(Solution Temp:955ºC
Cooling rate: 42 ºC/min
Initial Volume fraction: 0.274)

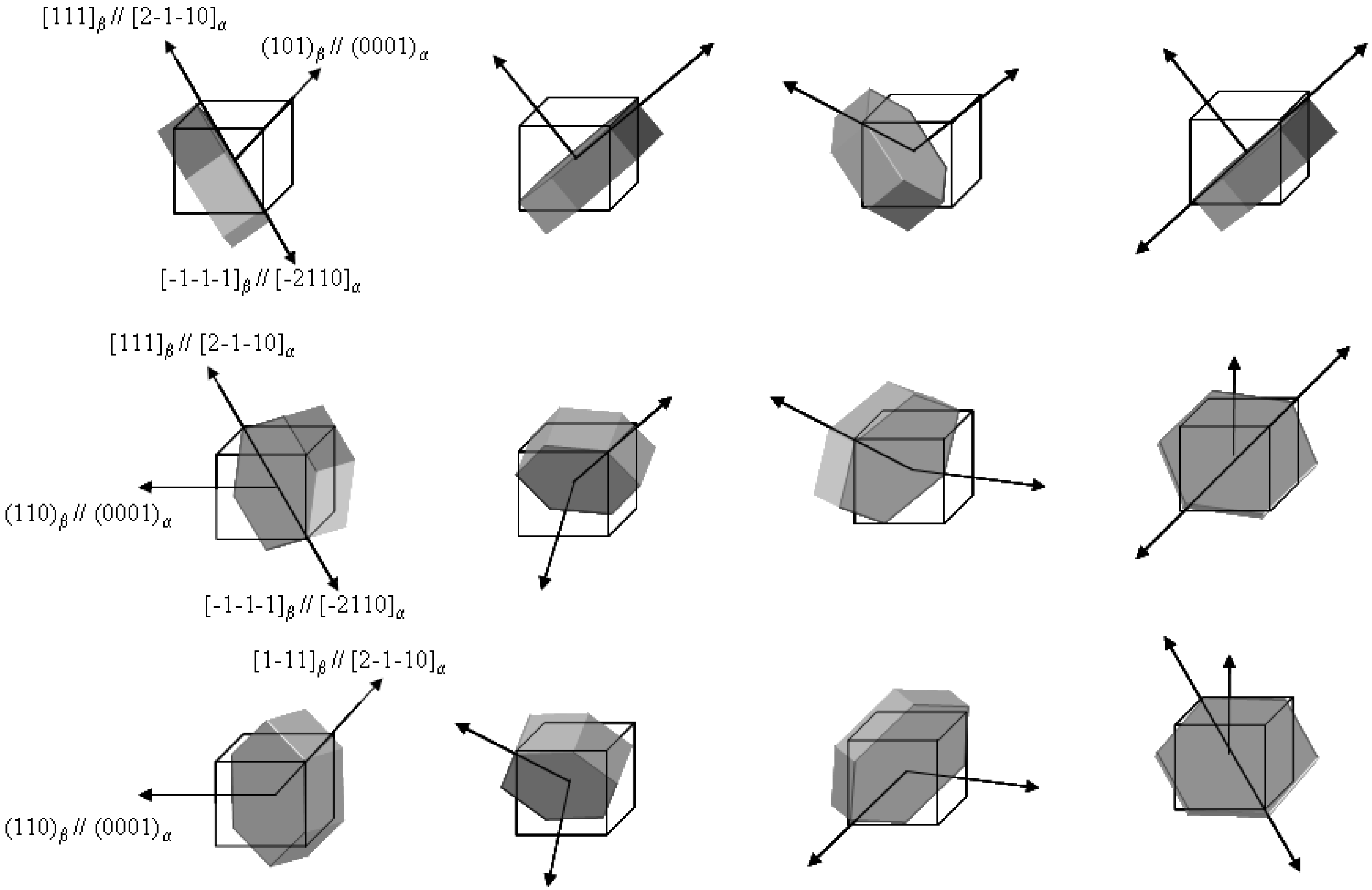
Ti 101: typical processed microstructures

Duplex



Crystallographic orientation of secondary alpha laths

Variant selection rules: 12 alpha-phase variants



Variant selection rules being incorporated

- All variants randomly selected
- Orientations with similar texture to primary alpha phase selected
- Orientations favored by slip activity in the beta phase selected

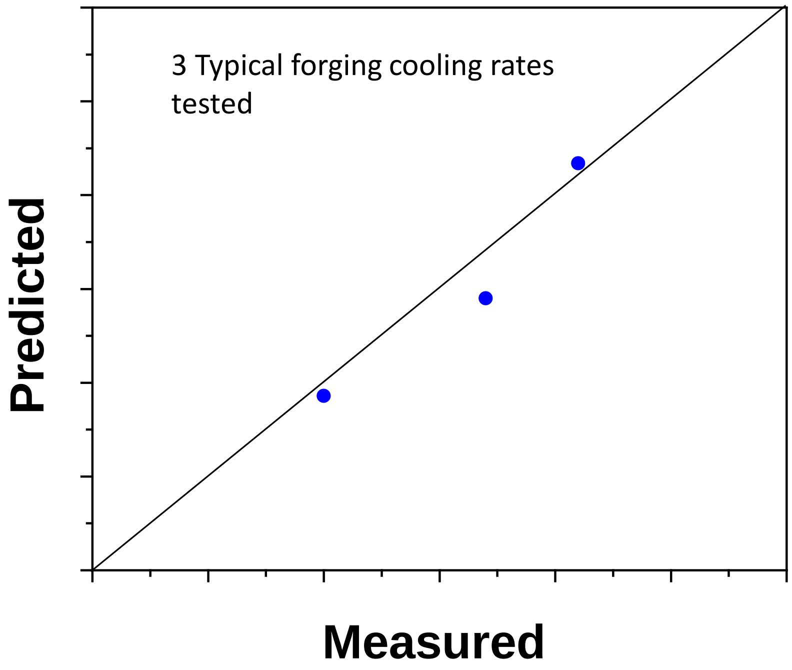
<u>Note:</u> User will have the ability to select which rule works the best based upon specific application and subsequent validation work to occur in later in Task 3 and in Task

Thickness of secondary alpha laths

Fast Acting Phase Field Model Integration

- Empirical equation developed based upon phase field results
- Equation then incorporated into DEFORM

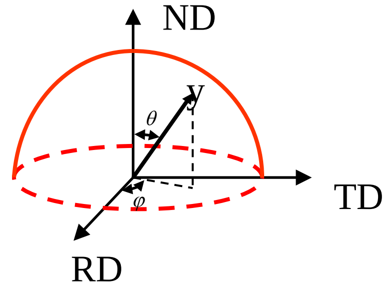
Secondary Alpha Lath Thickness



Incorporation of crystallographic texture into a neural net

Kearns Numbers

A simple quantitative methodology to incorporate crystallographic texture into a neural net database



$$f_{RD} = \frac{1}{N}\int_0^{2\pi}\int_0^{\pi/2} P(\varphi,\theta)\cos^2\varphi\sin^3\theta d\theta d\varphi$$

$$f_{TD} = \frac{1}{N}\int_0^{2\pi}\int_0^{\pi/2} P(\varphi,\theta)\sin^2\varphi\sin^3\theta d\theta d\varphi$$

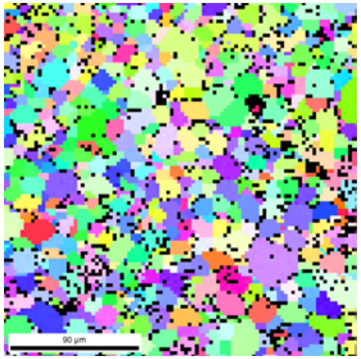
$$f_{ND} = \frac{1}{N}\int_0^{2\pi}\int_0^{\pi/2} P(\varphi,\theta)\cos^2\theta\sin\theta d\theta d\varphi$$

$$N = \int_0^{2\pi}\int_0^{\pi/2} P(\varphi,\theta)\sin\theta d\theta d\varphi$$

DEFORM Verification on a Randomly Oriented Data Set

Direction	Theoretical Value	Deform
ND	0.333	0.333
RD	0.333	0.333
TD	0.333	0.333

Kearns Number Validation for an EBSD Data Set



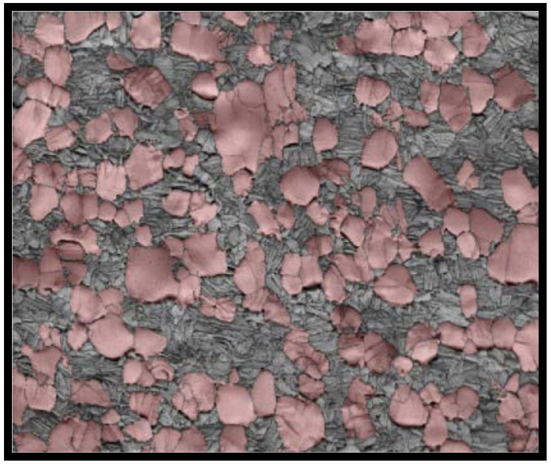
Direction	HKL	TiKn[TM]	Deform
ND	0.652	0.650	0.649
RD	0.293	0.294	0.294
TD	0.055	0.056	0.056

Note: Data set with un-indexed points selected on purpose

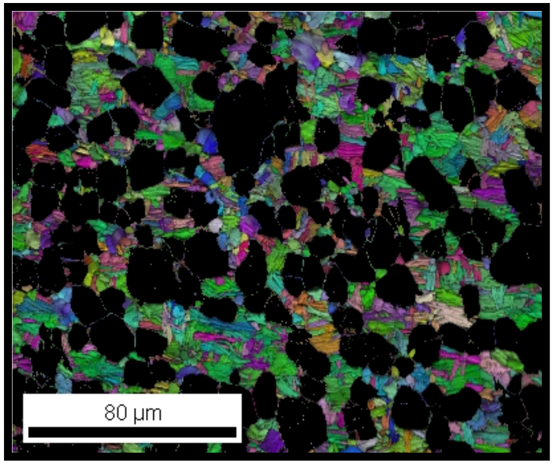
Rolls-Royce

Separation of α and α_s EBSD Data

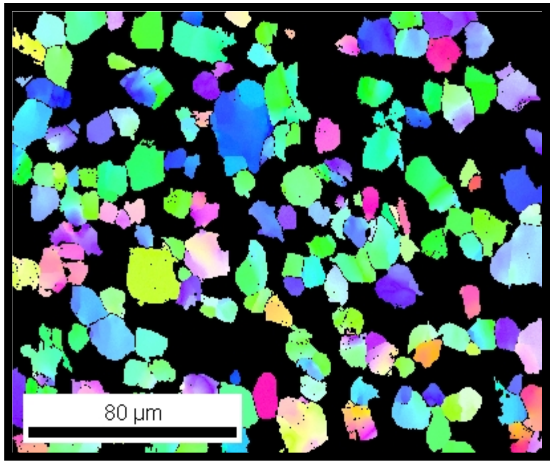
Using TiSeg™ to identify and segment various constituents



IQ map of α_p+α_s



IQ +IPF map of α_s

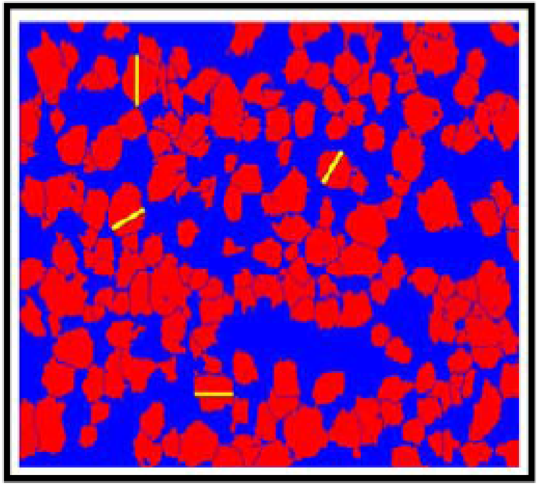


IPF map of α_p

- **Applying various filters to the OIM dataset of electropolished sample.**
- **Auto segmentation with accuracy ~90-95% in *2.0 seconds*.**
- **Followed by manual inspection for fine tuning.**

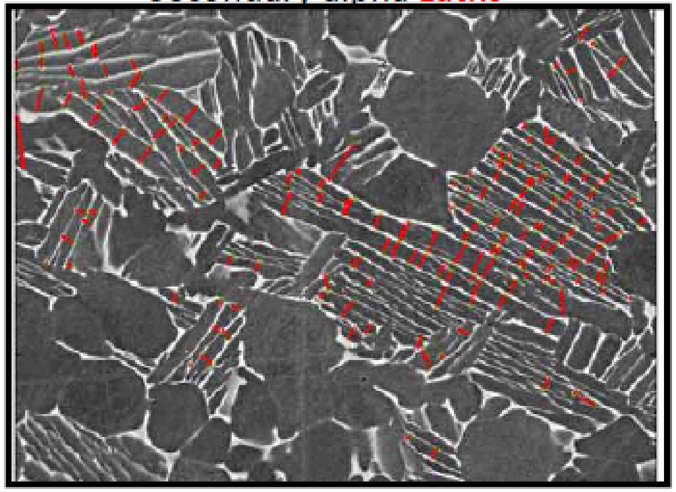
Measurement of microstructure features for neural net

Primary alpha **Grains**



From Segmented EBSD data, Chords were *automatically* plotted. CLD were calculated. Various statistics were extracted (e.g. Median, Mean, Max, Min, STDV,....etc)

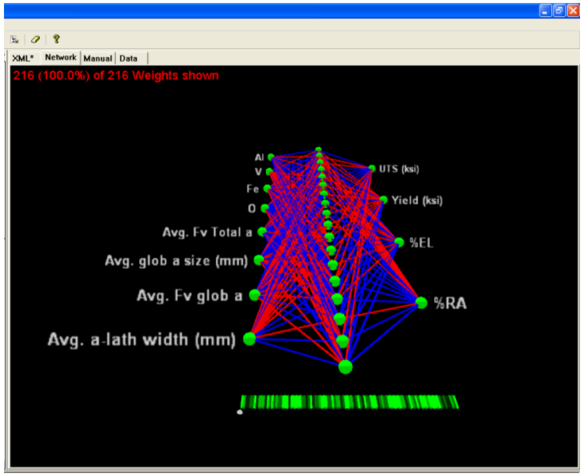
Secondary alpha **Laths**



From Segmented EBSD data or BSE images, Chords were *automatically* plotted. CLD were calculated. Various statistics were extracted (e.g. Median, Mean, Max, Min, STDV,....etc)

Commercial neural net model integration strategy

PatternMaster Software



Possible output formats of trained NN

Microsoft Excel Spreadsheet

C, Fortran executable

Selected output for MAI program and DEFORM integration

Conclusions

- **In early 2014 the current MAI Ti modeling program will enable the US aerospace industry to predict location specific properties in their Ti-6Al-4V forgings including:**
  - **Mechanical properties**
    - **YS, UTS, %El, RA**
  - **Microstructure**
    - **Prior beta grain size**
    - **Primary alpha size and volume fraction**
    - **Secondary alpha lath size**
    - **Colony alpha lath thickness**
  - **Crystallographic texture**
    - **Primary alpha**
    - **Secondary alpha**
    - **Beta phase**
    - **Colony alpha**