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Modeling of the dynamic inelasticity of poly- and single crystal tantalum under ramp wave loading*

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Outline

- Experimental observations of poly- and single crystal tantalum behavior under ramp wave loading.

- Objectives and approach.

- Dislocation-mechanics based continuum material model for polycrystal.

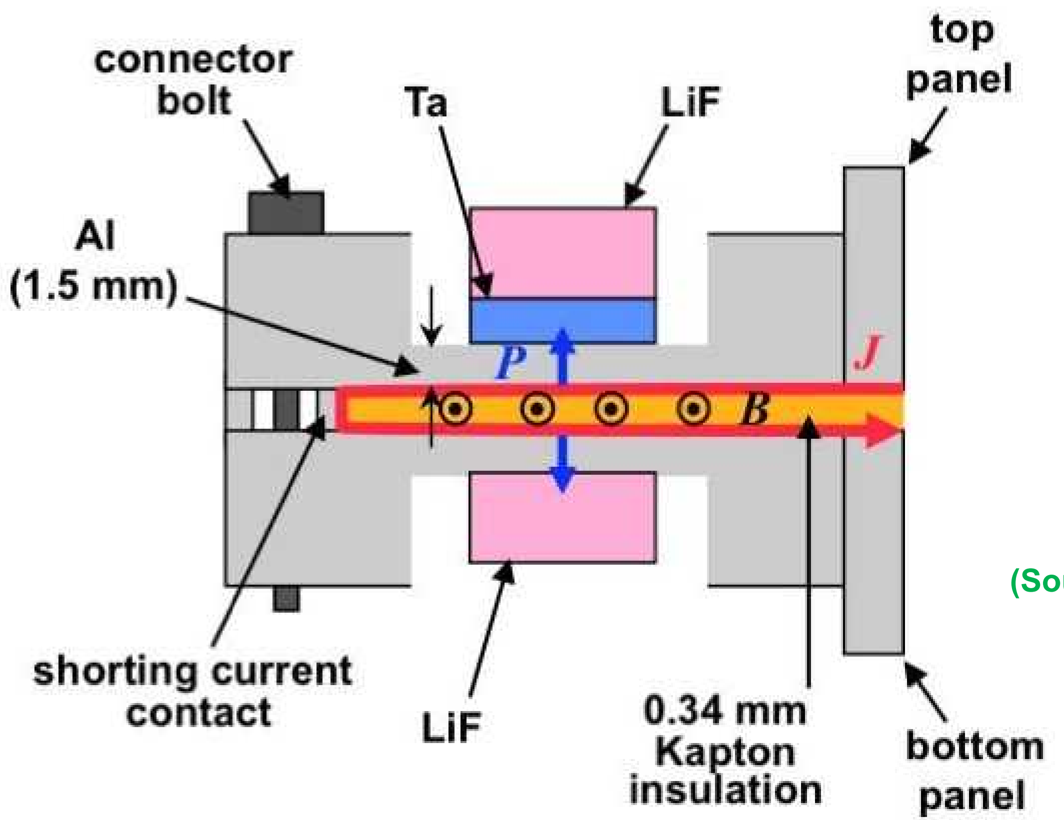
- Simulation of the single crystal experiments and insights gained from the simulation.

- Extension of the polycrystal model to single crystals.

- Simulation of the single crystal experiments and insights gained from the simulation.

- Conclusion.

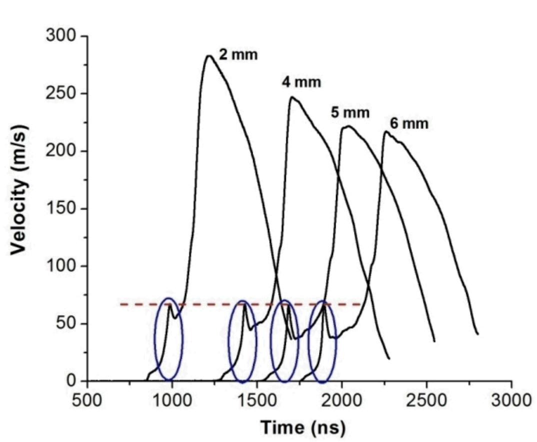
Configuration Of The Ramp Wave Experiments On Veloce



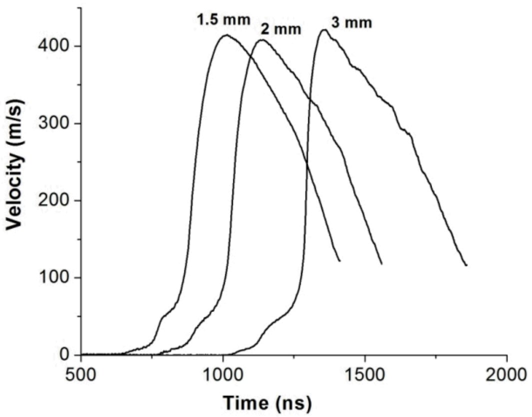
(Source: Ao et al. Rev. Sci. Instr. 2008)

generate a structured wave with finite risetime in the very high stress regime

Polycrystal Tantalum Under Ramp Wave Loading



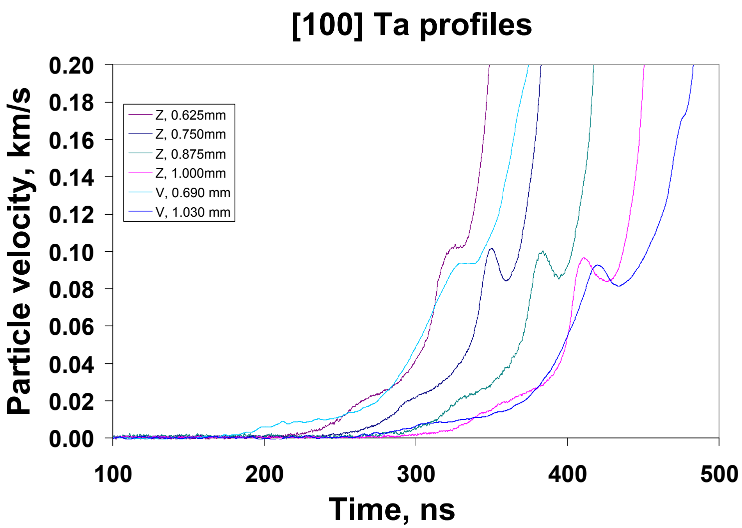
Annealed

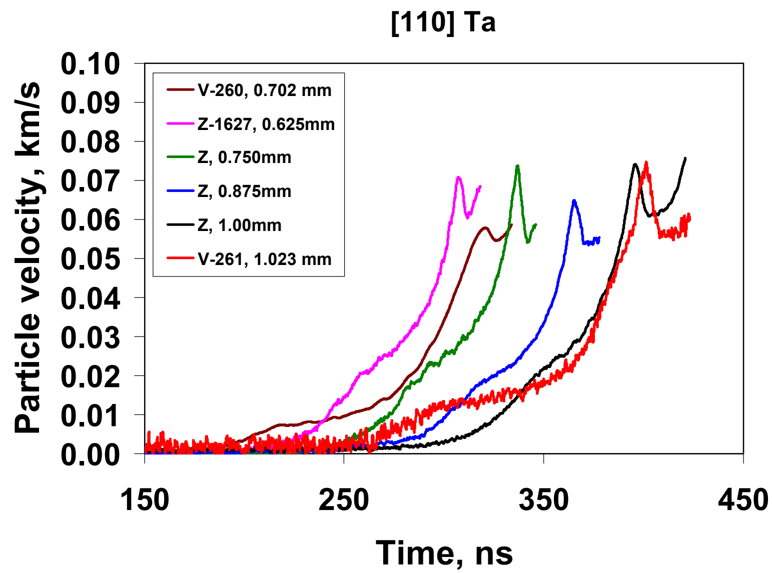


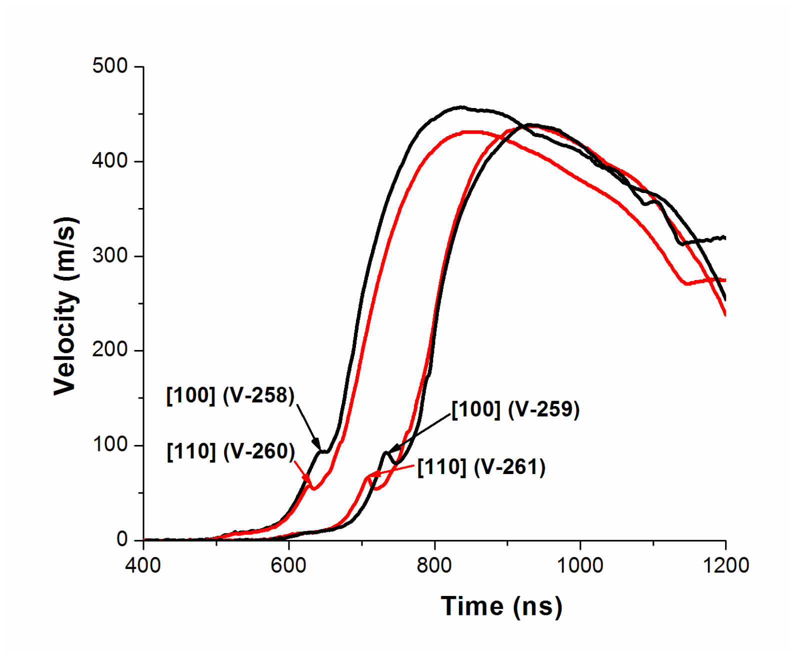
Cold-Rolled (26%)

- **Annealed samples**:
  - **Elastic precursor showed a pronounced overshoot followed by a significant velocity drop or stress relaxation**
  - **The extent of the velocity drop increased with the sample thickness.**
  - **precursor amplitude showed very little attenuation, even with the significant stress relaxation behind the precursor**
- **Cold-Rolled**:
  - **More dispersed elastic precursor.**
  - **no rapid velocity drop or stress relaxation was observed behind the precursor**

Single Crystal Tantalum Under Ramp Wave Loading

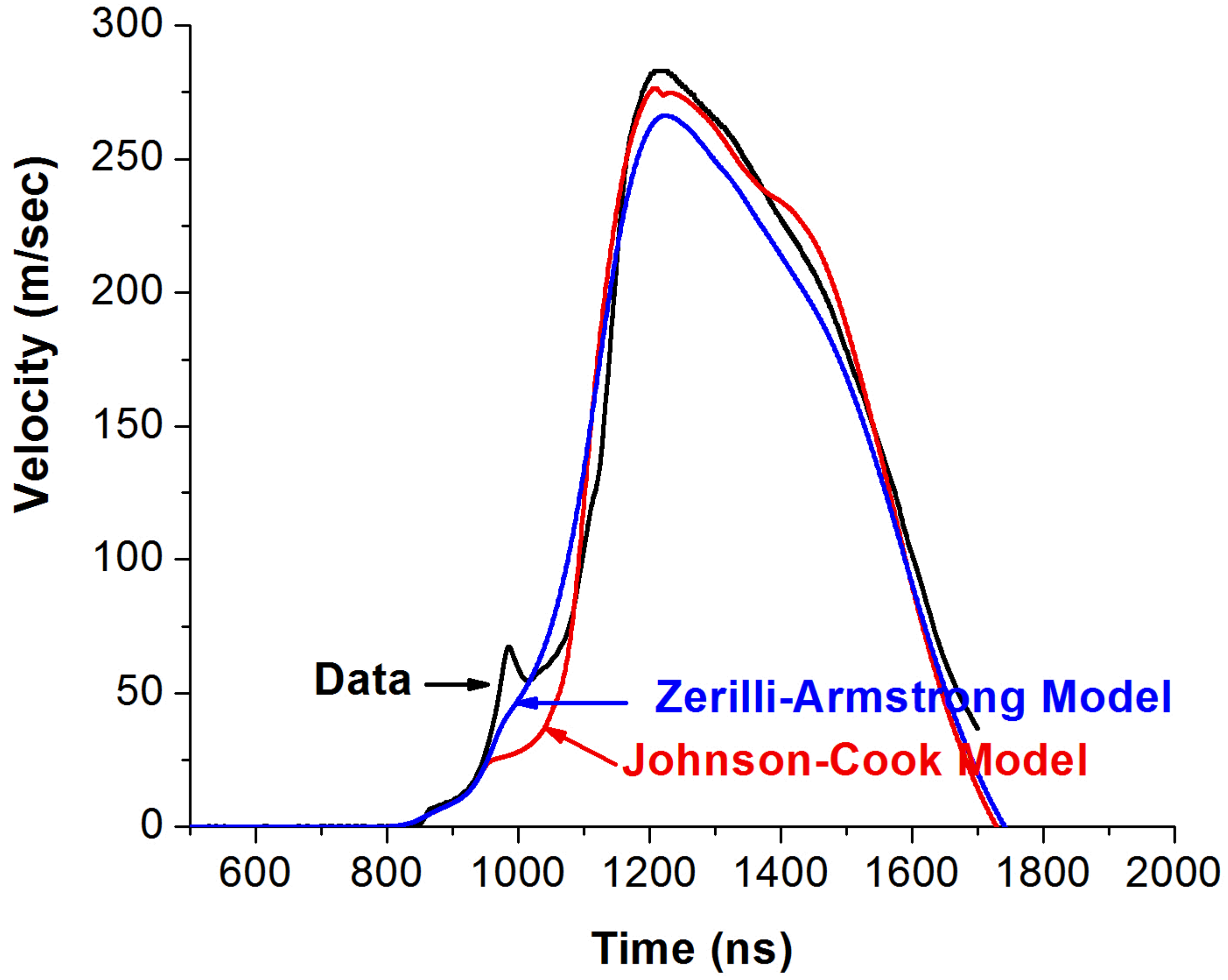






- Similar elastic precursor behavior as polycrystal.
- Strong orientation dependence
- [100] orientation showed slight decay of the precursor , but no apparent trend for [110] orientation.
- [100] orientation is more rate sensitive than [110].

Comparison of Annealed Polycrystal With Some Existing Models



Objectives and Approach

Objectives:

- To gain insights into the mechanical behavior of tantalum, particularly the elastic precursor behavior, and their implication on the deformation mechanisms for tantalum.
- To gain an understanding of the dynamic inelasticity of poly- and single crystal tantalum, including the material strength and its evolution.

Approach:

- Develop a constitutive model that captures the material features observed experimentally.
- Use numerical simulation to gain additional insight into the inelastic behavior of tantalum.

Thermomechanical Constitutive Relation

$$\dot{\sigma}_{ij}^{e} = B_{ijkl}\dot{\varepsilon}_{kl}^{e} - \rho\Gamma_{ij}\theta\dot{s} = B_{ijkl}(\dot{\varepsilon}_{kl} - \dot{\varepsilon}_{kl}^{p}) - \rho\Gamma_{ij}\theta\dot{s}$$

$$\left(B_{ijkl} = \left.\frac{\partial\sigma_{ij}}{\partial\varepsilon_{kl}^{e}}\right|_{s}, \quad \Gamma_{ij} = -\frac{1}{\rho\theta}\left.\frac{\partial\sigma_{ij}}{\partial s}\right|_{\varepsilon_{ij}^{e}} \right)$$

$$\dot{\theta} = -\theta\Gamma_{ij}\dot{\varepsilon}_{ij}^{e} + (\theta / C_{v})\dot{s} = -\theta\Gamma_{ij}(\dot{\varepsilon}_{ij} - \dot{\varepsilon}_{ij}^{p}) + (\theta / C_{v})\dot{s}$$

$$\dot{s} = \frac{1}{\rho\theta}(\sigma_{ij}^{'e}\dot{\varepsilon}_{ij}^{p} - q_{i,i})$$

$$q_{i} = -k\theta_{,i}$$

$$\dot{\gamma} = \dot{\gamma}_{mech} + \dot{\gamma}_{con}$$

$$\dot{\gamma}_{mech} = \frac{ds}{dt} - (-\frac{1}{\rho\theta}q_{i,i}) = \frac{\sigma_{ij}^{e'}\dot{\varepsilon}_{ij}^{p}}{\rho\theta} \geq 0$$

$$\dot{\gamma}_{con} = -\frac{1}{\rho\theta^{2}}q_{i}\theta_{,i} \geq 0$$

Strength Model

$$\dot{\sigma}'_{ij} = 2G\dot{\varepsilon}^{e}_{ij}{}' = 2G(\dot{\varepsilon}'_{ij} - \dot{\varepsilon}^{p}_{ij})$$

$$\dot{\varepsilon}^{p}_{ij} = \dot{\bar{\varepsilon}}^{p}(\sigma'_{ij} / |\sigma'_{ij}|)$$ **and** $$\dot{\bar{\varepsilon}}^{p} = A[|\sigma'_{ij}| - \sigma_{th})]^{1.5}$$

$$\dot{\bar{\varepsilon}}^{p} = (\frac{2}{3}\dot{\varepsilon}^{p}_{ij}\dot{\varepsilon}^{p}_{ij})^{1/2}$$: effective plastic strain rate

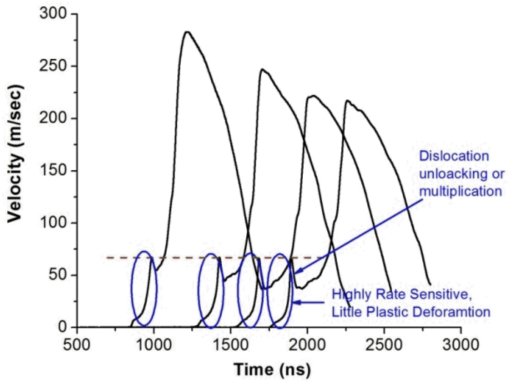
$$|\sigma'_{ij}| = (\frac{3}{2}\sigma'_{ij}\sigma'_{ij})^{1/2}$$: effective stress, a measure of material strength

$$G = G_0[1 + (\frac{G'_P}{G_0})\frac{P}{\eta^{1/3}} + (\frac{G'_T}{G_0})(T - T_0)]$$

$$\sigma_{th} = \sigma_{th_0}[1 + \beta(\bar{\varepsilon}^{p} + \bar{\varepsilon}^{p}_{i})]^{n}[1 + (\frac{G'_P}{G_0})\frac{P}{\eta^{1/3}} + (\frac{G'_T}{G_0})(T - T_0)]$$

(Steinberg, Cochran, and Guinan, JAP, 1980)

Association of The Rate Eqn. with Dislocation Motion



- **Little decay of precursor implies little plastic deformation during precursor loading**
- **Dislocation unlocking or multiplication at the precursor tip.**

Dislocation model (Orowan Eqn.):

$\dot{\gamma}^p = b\rho_m v$ where

- $\dot{\gamma}^p$: plastic strain rate;
- b : Burgers vector;
- ρ_m : mobile dislocation density;
- v : stress dependent dislocation velocity

$$\dot{\bar{\varepsilon}}^p = A[|\sigma'_{ij}| - \sigma_{th})]^{1.5} = b\rho_m\{c[|\sigma'_{ij}| - \sigma_{th})]^{1.5}\}$$

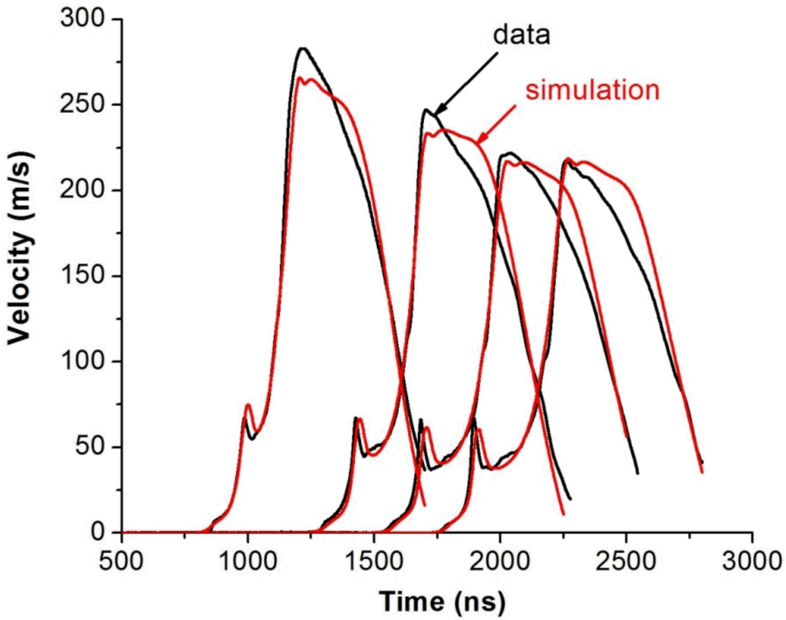
where

$\rho_m = f\rho_t$ with ρ_t being the total dislocation density

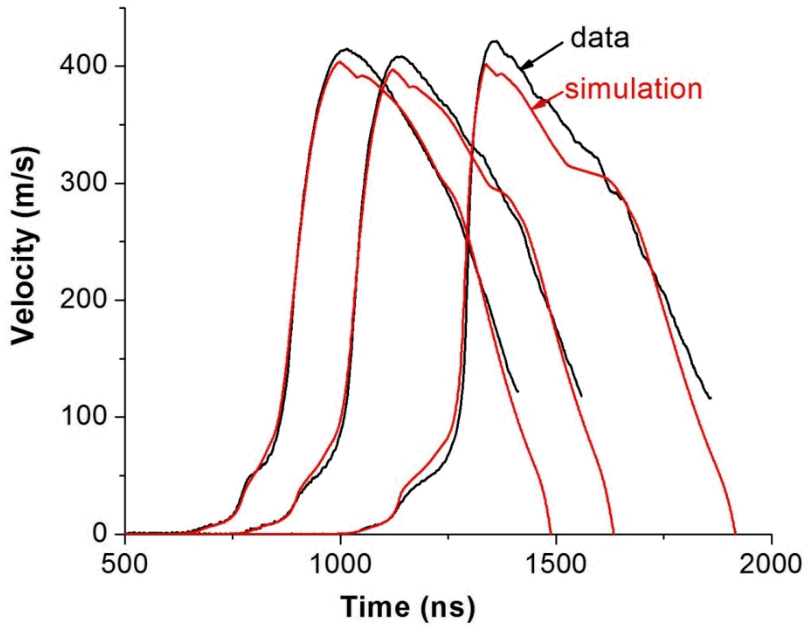
$\rho_t = \rho_0 + C(\bar{\varepsilon}^p)^a$ (Hahn, Acta Met. 1962)

$f = f_i + (f_f - f_i)(1 - e^{-\lambda\bar{\varepsilon}^p})$ (Yoshida et. al., IJP, 2008)

Simulated Polycrystal Velocity Histories



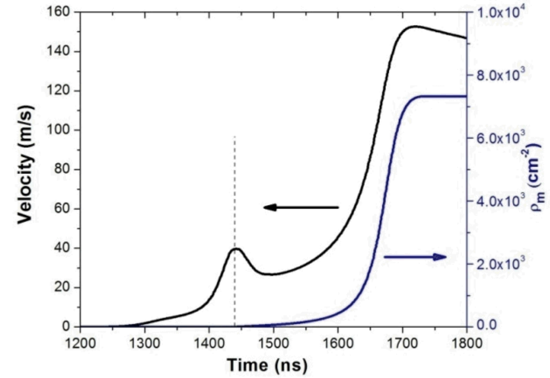
Annealed

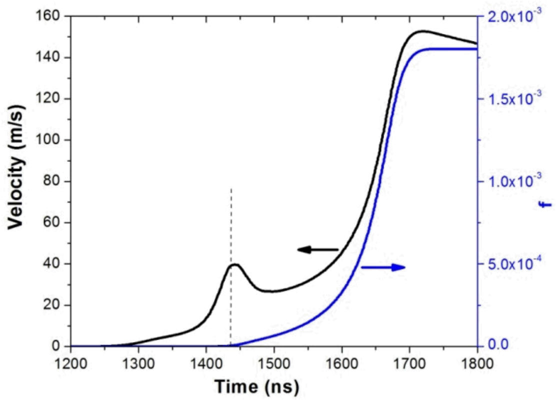


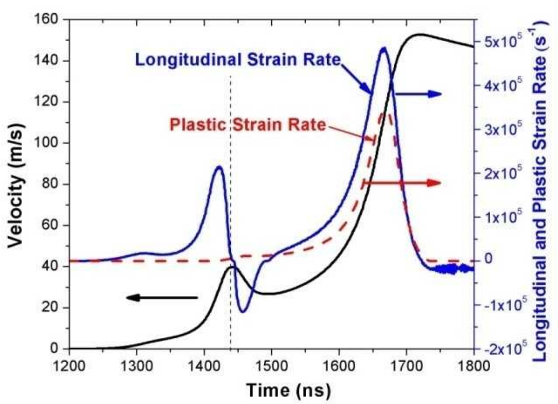
Cold-Rolled (26%)

Annealed vs Cold Rolled

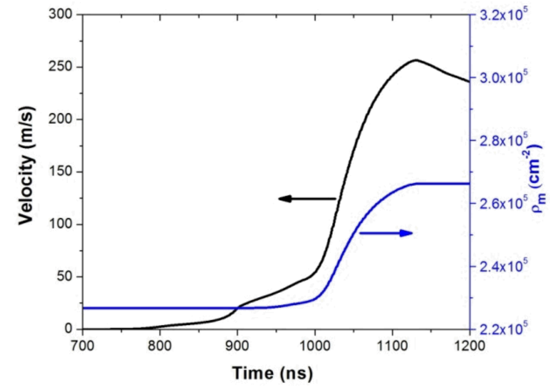
Annealed

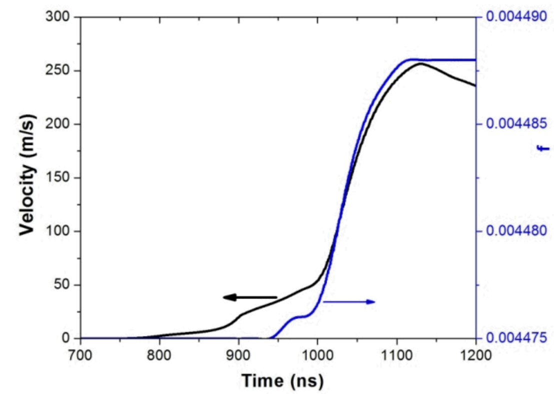


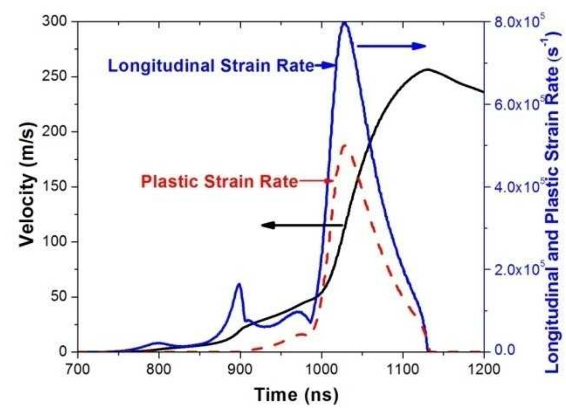




Cold-Rolled

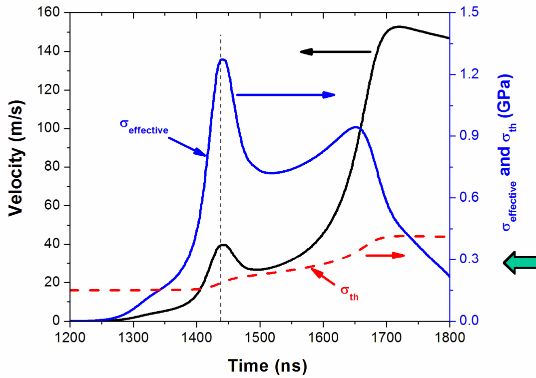




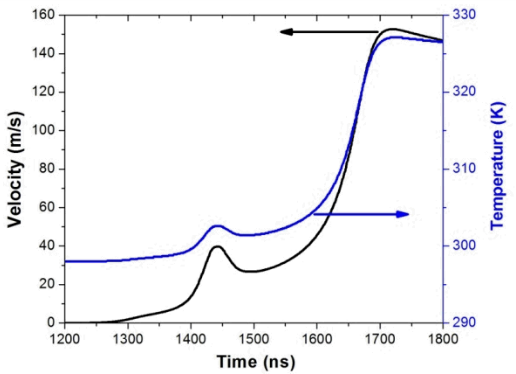


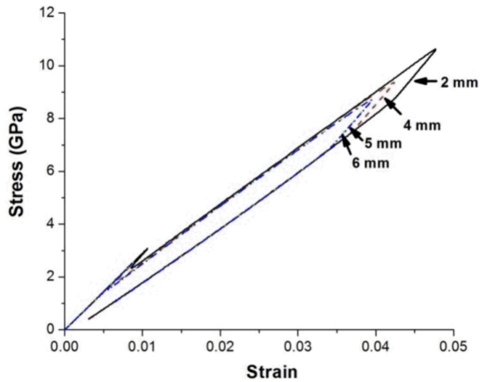
Annealed vs Cold Rolled

Annealed

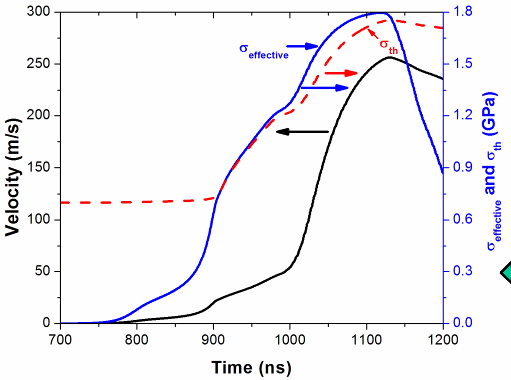


highly rate sensitive response

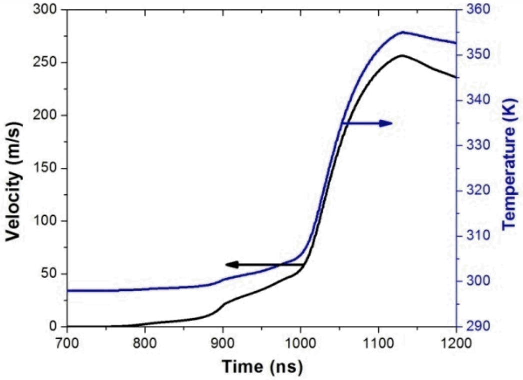


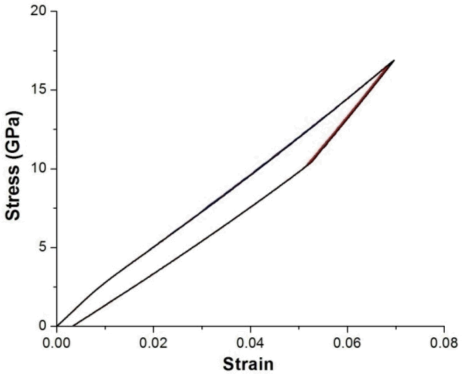


Cold-Rolled



less rate sensitive response





Simulation of Single Crystal Tantalum With Polycrystal Model

- **Use continuum model with different material constants for different orientations to describe the single crystal behavior.**

- **The model is used as a data analysis tool to estimate the material properties and their evolution.**

$$\dot{\bar{\varepsilon}}^p = A[|\sigma'_{ij}| - \sigma_{th})]^{1.5} = b\rho_m\{c[|\sigma'_{ij}| - \sigma_{th})]^2\} \quad (\dot{\gamma}^p = b\rho_m v)$$

where $\rho_m = f\rho_t$ with ρ_t being the total dislocation density

$$\rho_t = \rho_0 + C(\bar{\varepsilon}^p)^a$$ (Hahn, Acta Met. 1962)

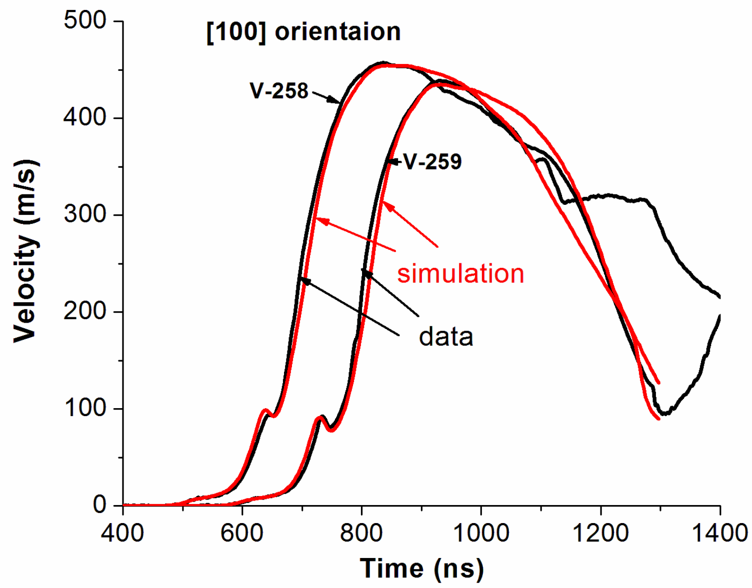
$$f = f_i + (f_f - f_i)(1 - e^{-\lambda\bar{\varepsilon}^p})$$ (Yoshida et. al., IJP, 2008)

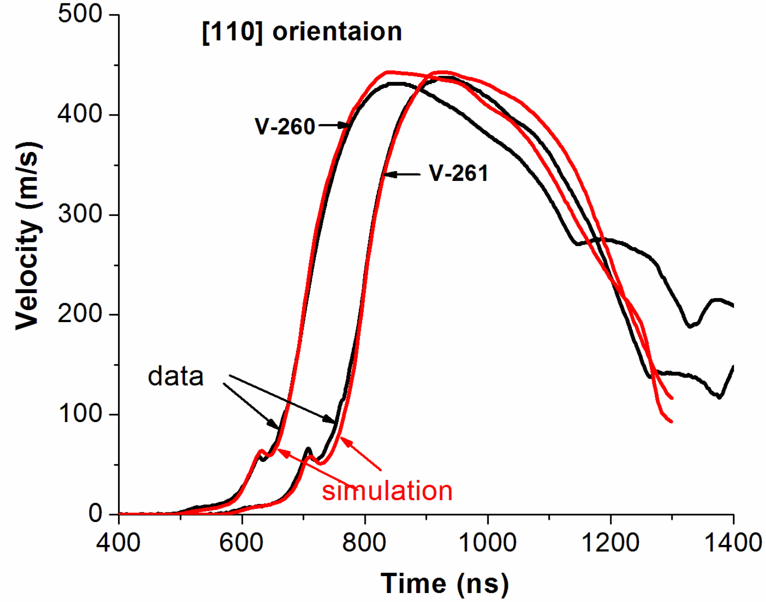
- **All the material constants are kept the same as for polycrystal except for λ**

- $\lambda = 25$ **for [100]; and** $\lambda = 60$ **for [110] orientation**

- **Smaller λ results in a more rate sensitive beahvior**

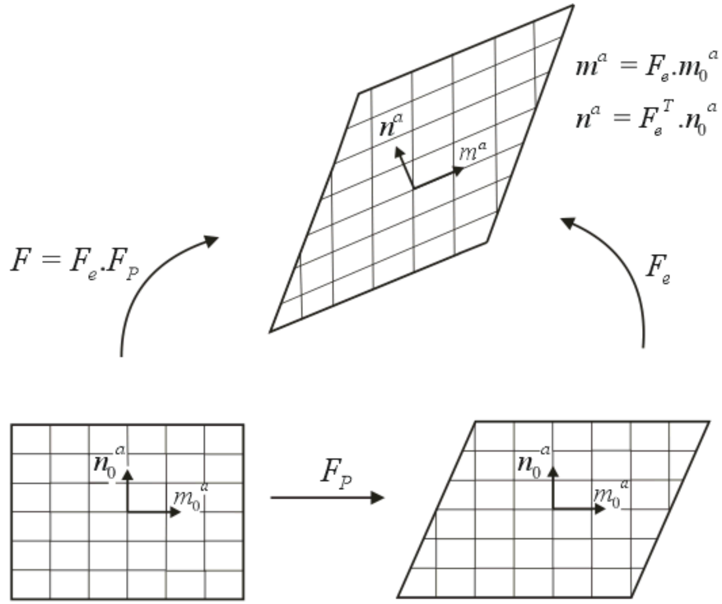
Simulation of Single Crystal Tantalum With Polycrystal Model





What is the physical justification for different rate sensitivity for different orientations?

Single Crystal Model - Kinematics



$$\tau^{\alpha} = \underline{\mathrm{m}}_0^{\alpha} \cdot \underset{\sim}{C}^{e} \cdot \underset{\sim}{S} \cdot \underline{\mathrm{n}}_0^{\alpha}$$

$$\underset{\sim}{\bar{L}}^{p} = \sum_{\alpha} \dot{\gamma}^{\alpha} \underline{\mathrm{m}}_0^{\alpha} \otimes \underline{\mathrm{n}}_0^{\alpha}$$

Single Crystal Model – Constitutive Relation

$$\dot{\gamma}^{\alpha} = b\rho_m^{\alpha}\overline{v}^{\alpha} = b\rho_m^{\alpha}\{\beta[(\left|\tau^{\alpha}\right| - \tau_{th}^{\alpha}) / \tau_{th}^{\alpha}]^{\mu}\}$$

$$\rho_m^{\alpha} = f^{\alpha}\rho_t^{\alpha}$$

$$f^{\alpha} = f_0^{\alpha} + (f_s^{\alpha} - f_0^{\alpha})(1 - e^{-\lambda^{\alpha}\gamma^{\alpha}})$$

$$\rho_t^{\alpha} = \rho_{t0}^{\alpha} + \kappa(\gamma^{\alpha})^{\eta}$$

$$\tau_{th}^{\alpha} = \tau_0^{\alpha}(1 + \omega\gamma)^{\zeta}$$

Single Crystal Model – Slip Systems

Slip System Considered: {110}<111> and {112}<111>

{112}<111> possesses twinning/anti-twinning asymmetry

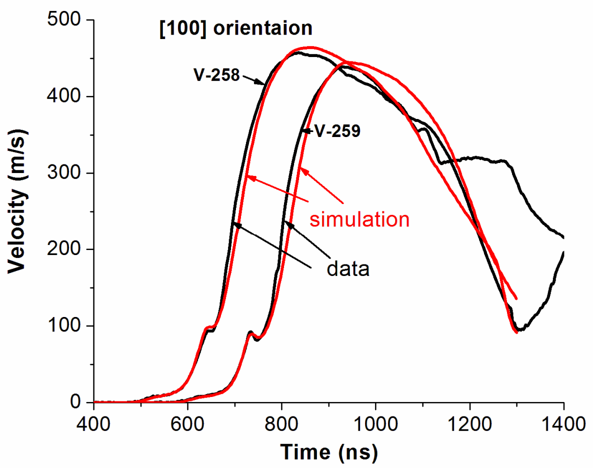
1	$(0\bar{1}1)[111]$	**13**	$(1\bar{2}1)[111]$
2	$(1\bar{1}0)[111]$	**14**	$(\bar{2}11)[111]$
3	$(10\bar{1})[111]$	**15**	$(11\bar{2})[111]$
4	$(01\bar{1})[\bar{1}11]$	**16**	$(\bar{1}1\bar{2})[\bar{1}11]$
5	$(\bar{1}0\bar{1})[\bar{1}11]$	**17**	$(211)[\bar{1}11]$
6	$(1\bar{1}0)[\bar{1}11]$	**18**	$(\bar{1}\bar{2}1)[\bar{1}11]$
7	$(011)[\bar{1}\bar{1}1]$	**19**	$(\bar{1}21)[\bar{1}\bar{1}1]$
8	$(\bar{1}10)[\bar{1}\bar{1}1]$	**20**	$(2\bar{1}1)[\bar{1}\bar{1}1]$
9	$(\bar{1}0\bar{1})[\bar{1}\bar{1}1]$	**21**	$(\bar{1}\bar{1}\bar{2})[\bar{1}\bar{1}1]$
10	$(0\bar{1}\bar{1})[1\bar{1}1]$	**22**	$(1\bar{1}\bar{2})[1\bar{1}1]$
11	$(10\bar{1})[1\bar{1}1]$	**23**	$(\bar{2}\bar{1}1)[1\bar{1}1]$
12	$(110)[1\bar{1}1]$	**24**	$(121)[1\bar{1}1]$

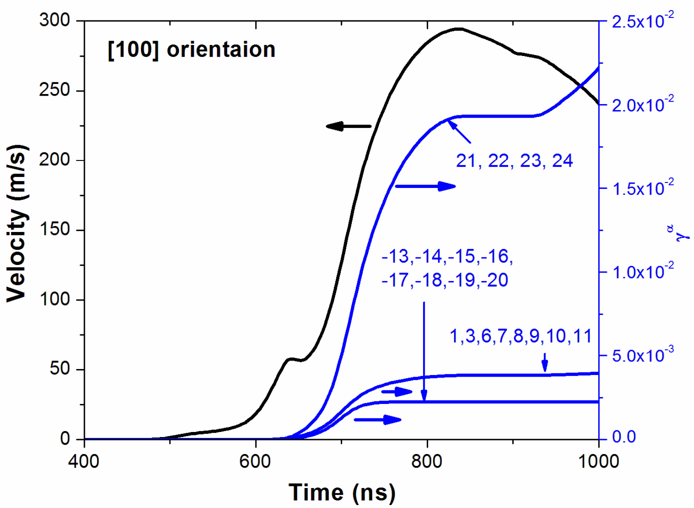
$\lambda = 15$ **for the above slip systems**

$\lambda = 50$ **for the {112}<111> system along the twinning direction**

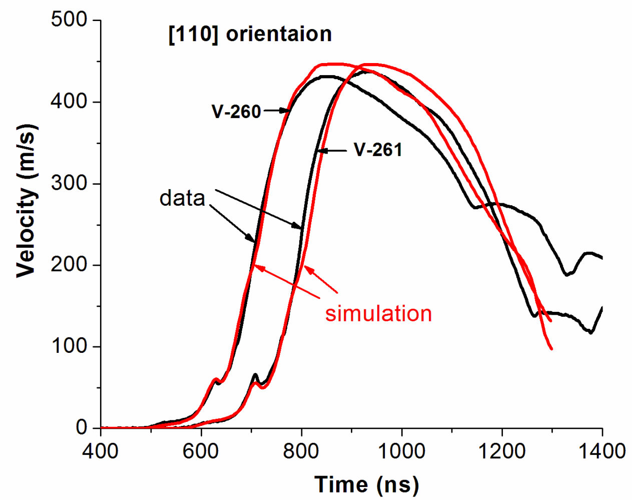
Simulation of Single Crystal Tantalum

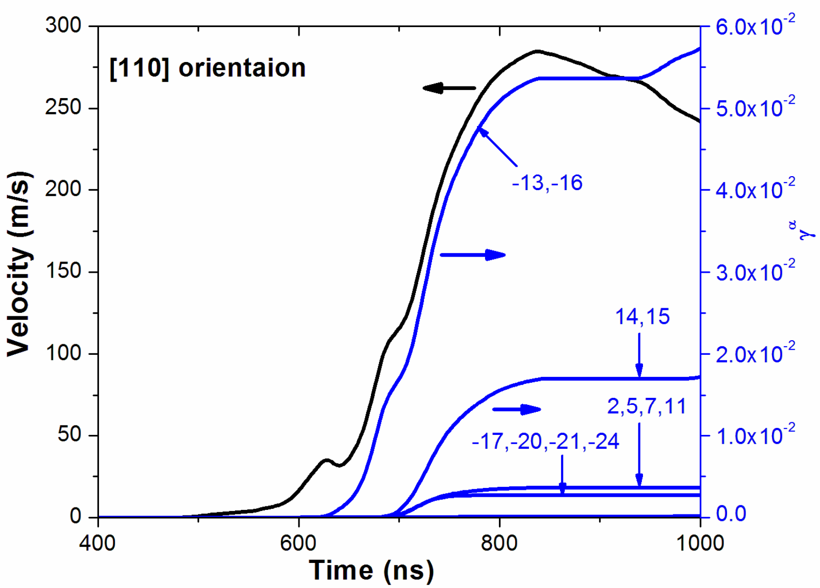
[100]



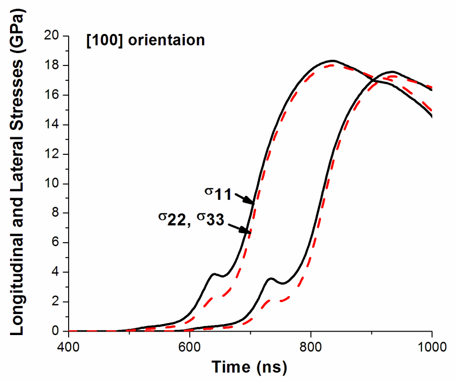


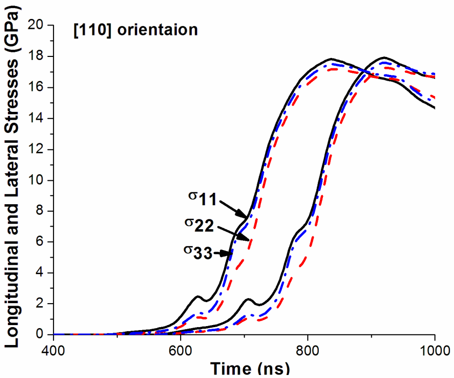
[110]

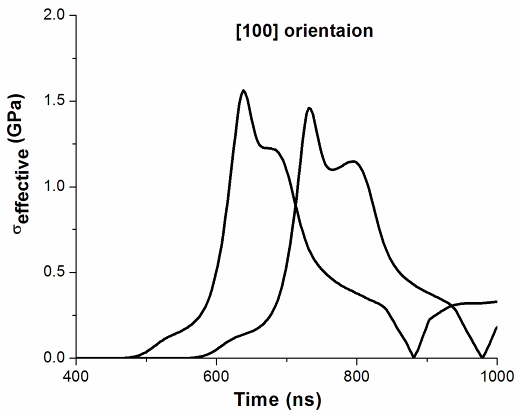


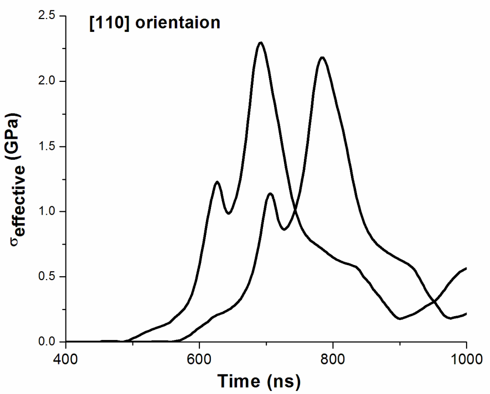


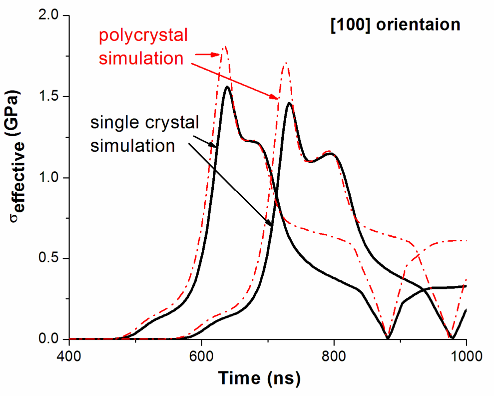
Simulation of Single Crystal Tantalum

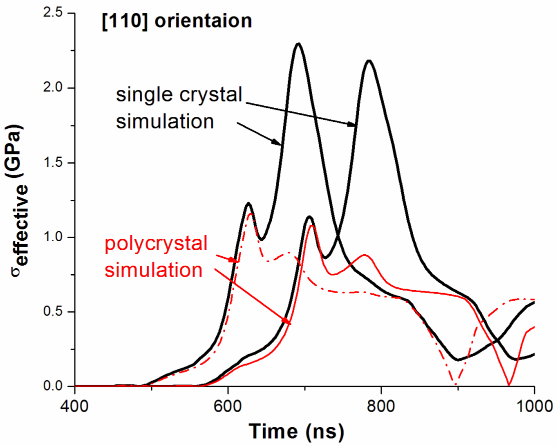




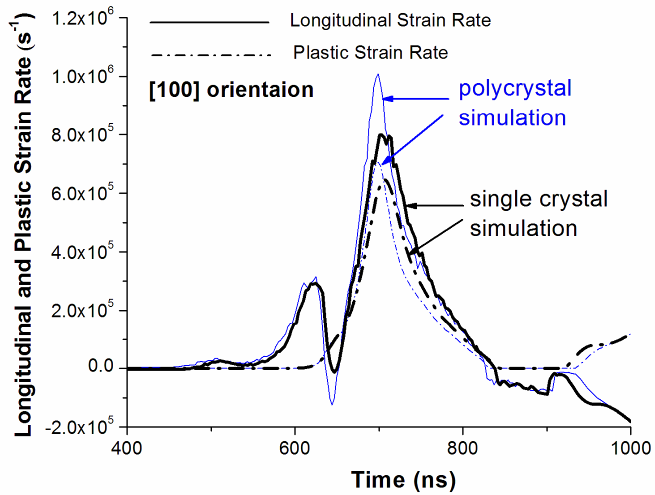


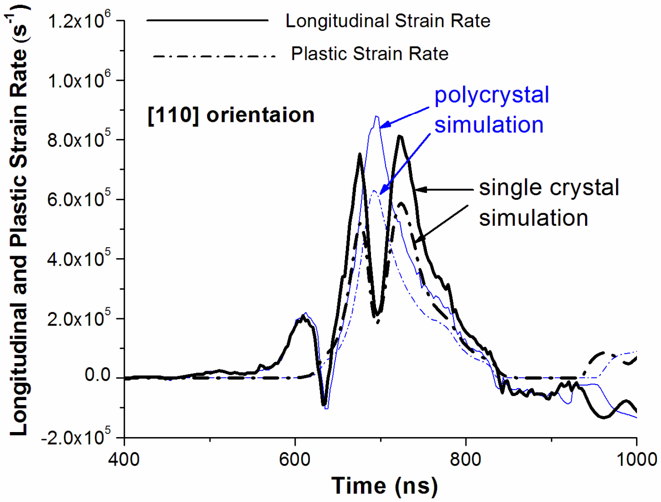


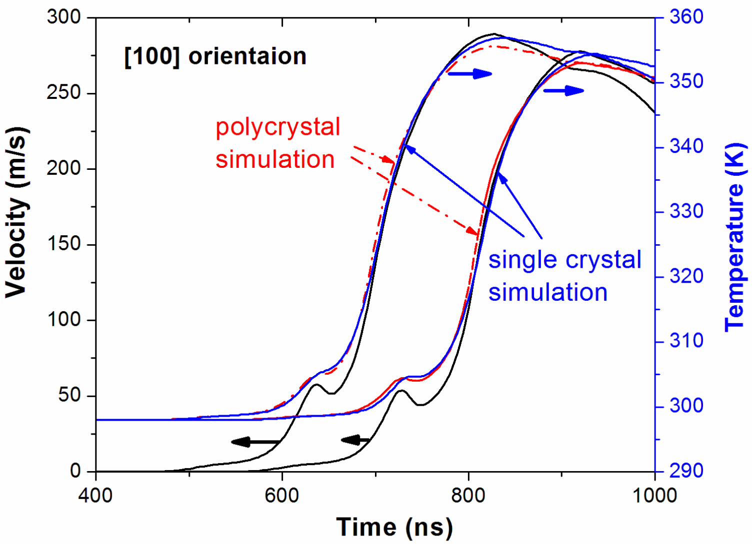


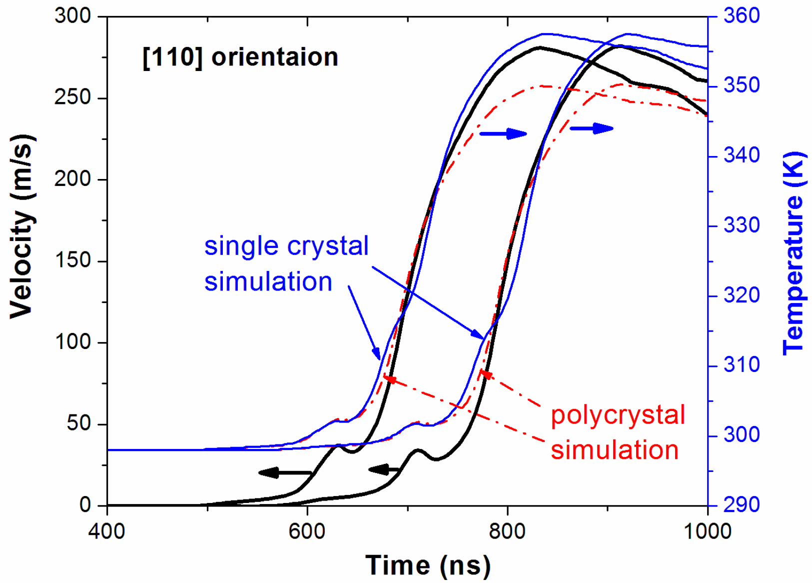


Simulation of Single Crystal Tantalum









Conclusions

- **A dislocation-mechanics based model yields consistent description of the behavior of both the poly- and single crystal tantalum under ramp wave loading.**

- **The various features of the observed tantalum behavior can be interpreted as a manifestation of the high rate sensitivity.**

- **Dislocation nucleation is used as a key mechanism for modeling the high rate sensitivity.**

- **On the microscopic level, the anisotropy of rate sensitivity is assumed to be attributed to the twinning/antitwinning asymmetry of the BCC crystals.**