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High Temperature Deformation Mechanisms in Ta2C

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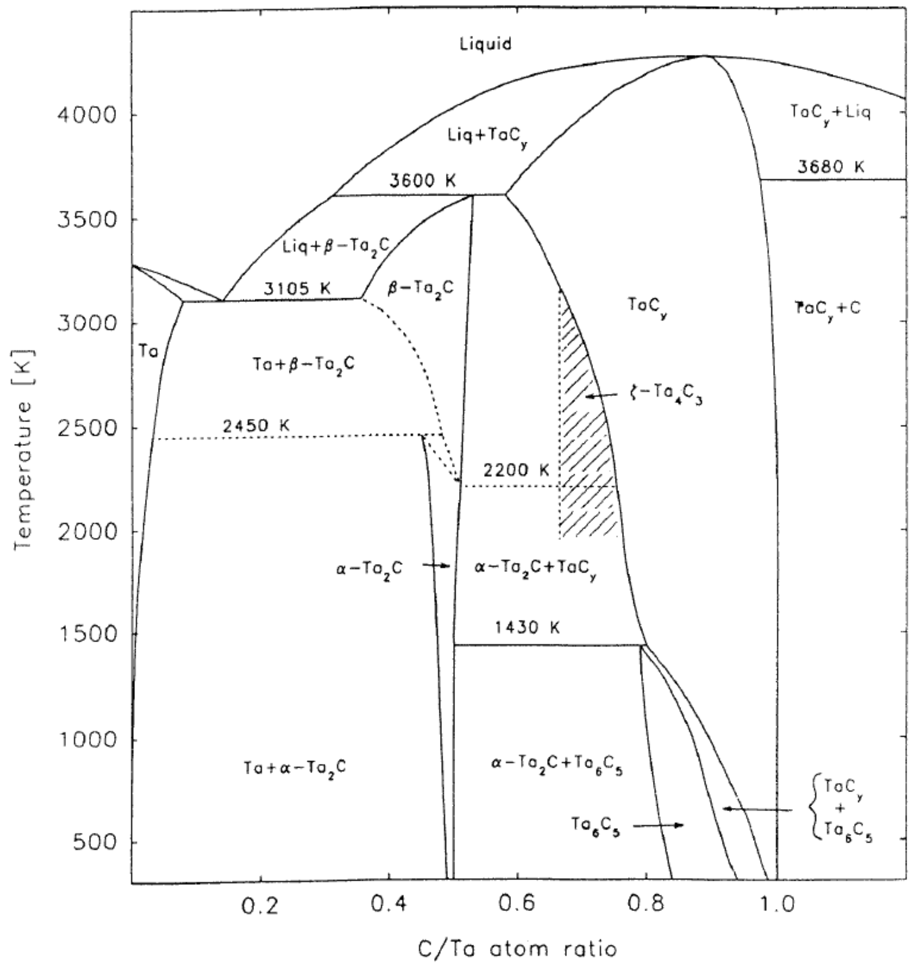
Tantalum – Tantalum Carbon Phase Diagram

- Carbon – Diamond Sublimes at 3800C
- TaC melts at 3900 C
- Ta4HfC5 melts at 4215 C

Tantalum Carbides are useful for high temperature structural applications.



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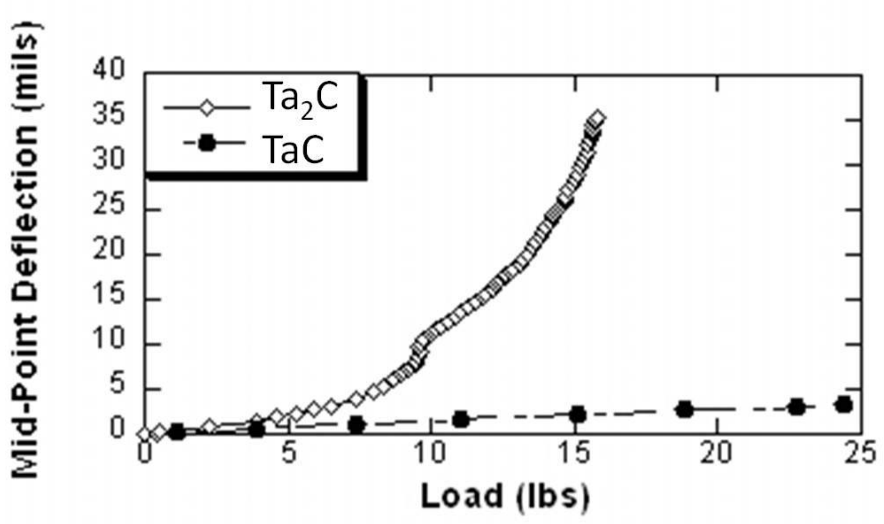
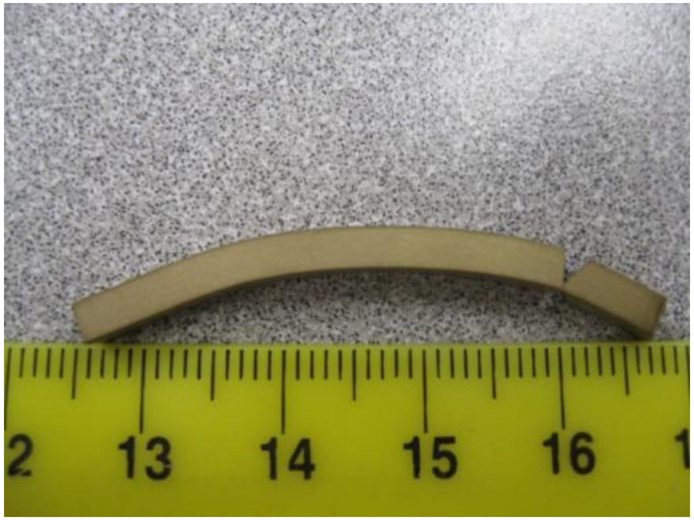
Plasticity in Tantalum Carbides



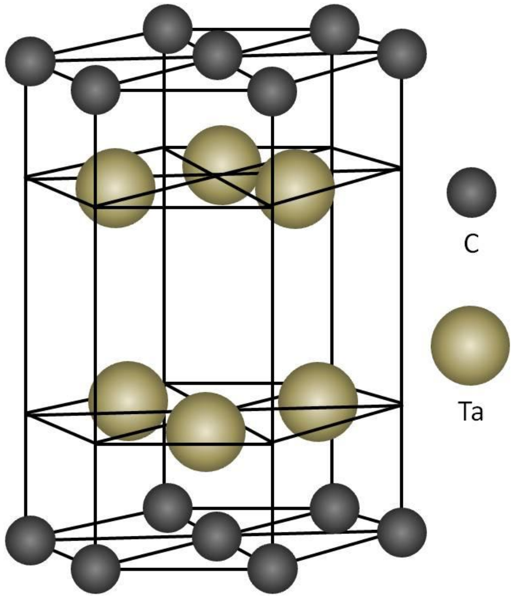


Ta2C shows significantly more plastic deformation than TaC at ~1930K

Ta2C

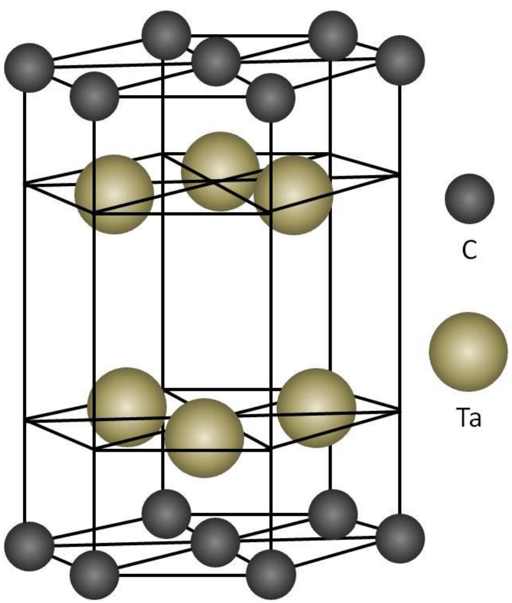
- Structure: C6 Anti-CdI2
- Space Group: P-3m1
- Point Group is -3m : Trigonal
- Stacking on the basal plane:
  - ABγABγABγ

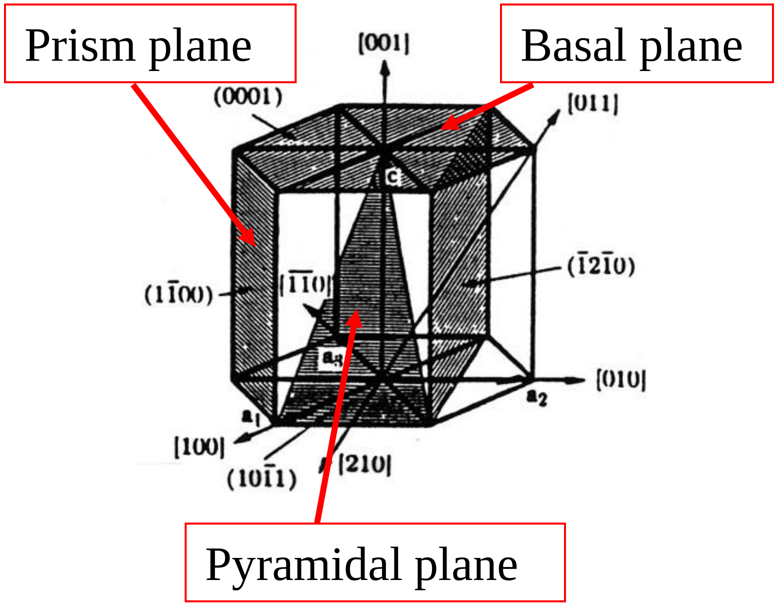
- Note that the stacking sequence involves the direct bonding of two tantalum layers.
- Exhibits mixed metallic-covalent bonding.



Slip in Hexagonal & Trigonal Crystals

- Perfect slip via 1/3<11-20>on {0001} (basal)
- Perfect slip via 1/3<11-20> on {10-10} (prism)
- Perfect slip via 1/3<11-23> on {11-22} {10-11}{hikl} (pyramidal and banal)
- Partial slip via 1/3<-1100> on {0001}





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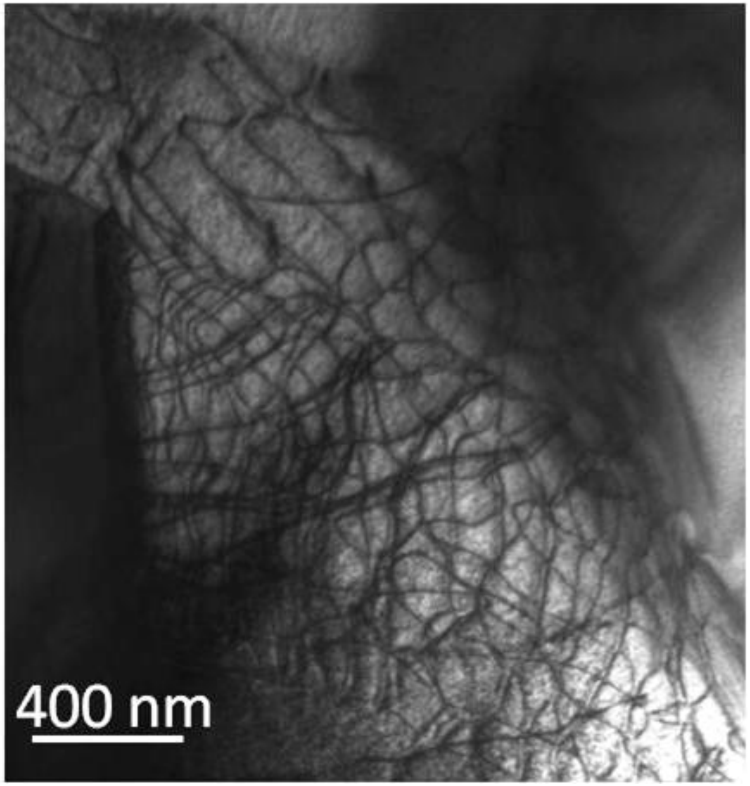
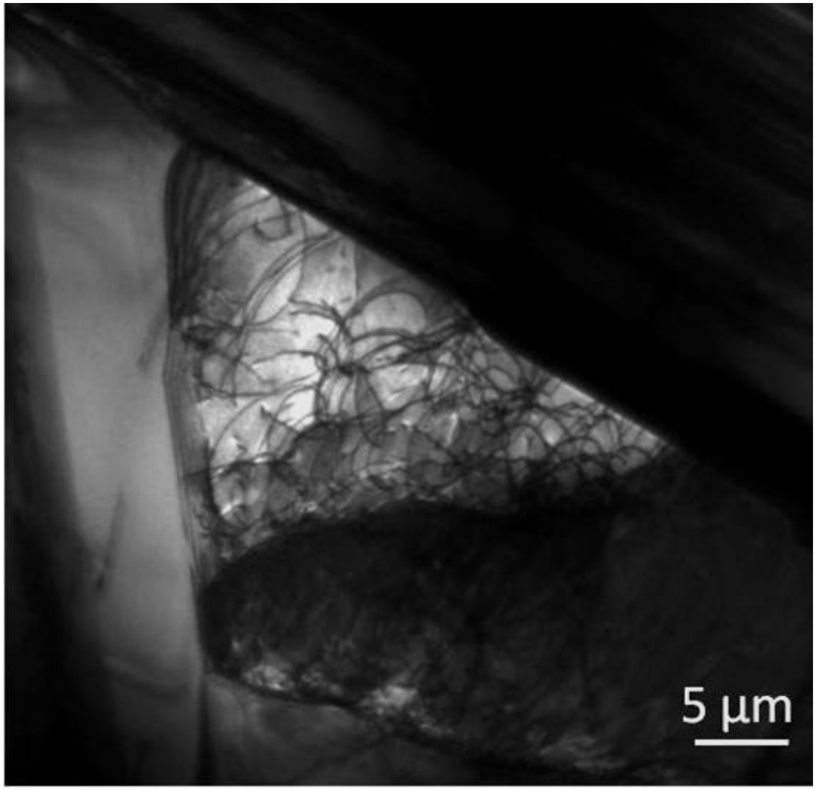
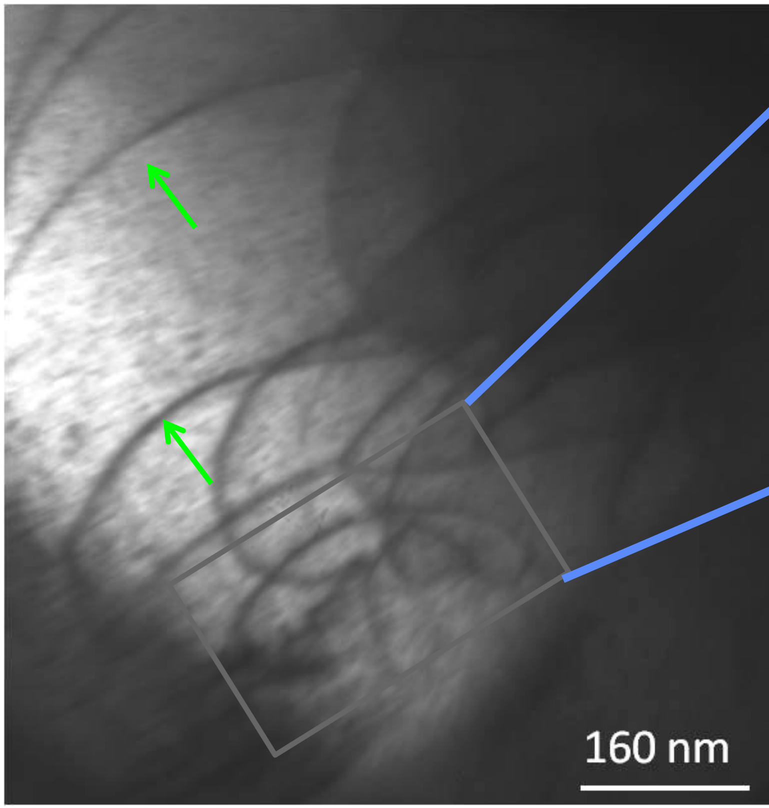
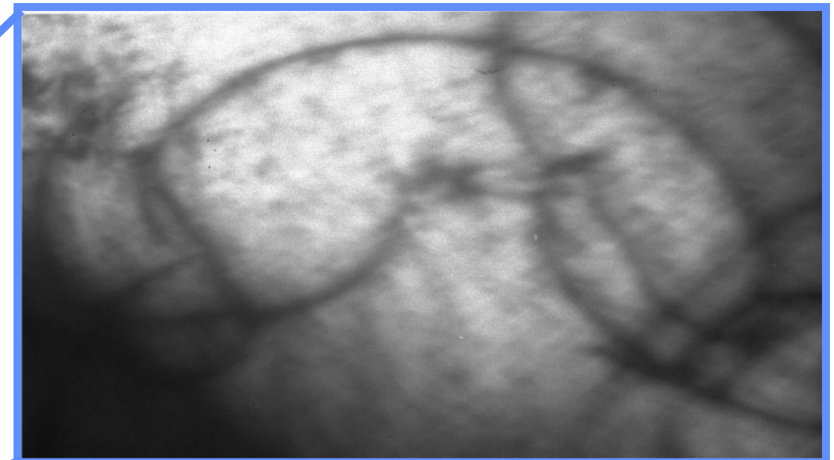
Dislocations in Ta2C

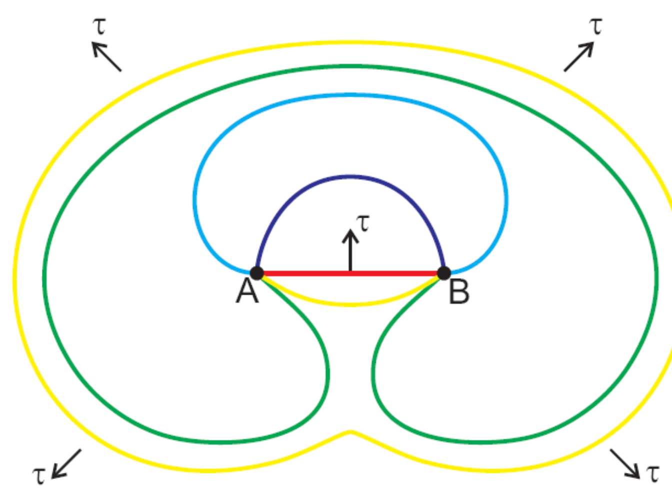




More Dislocations







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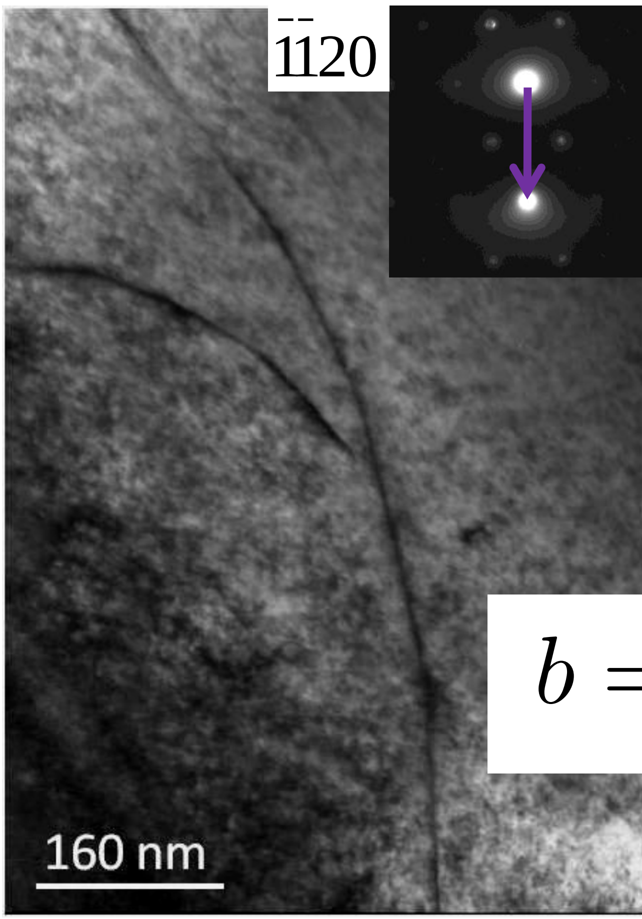
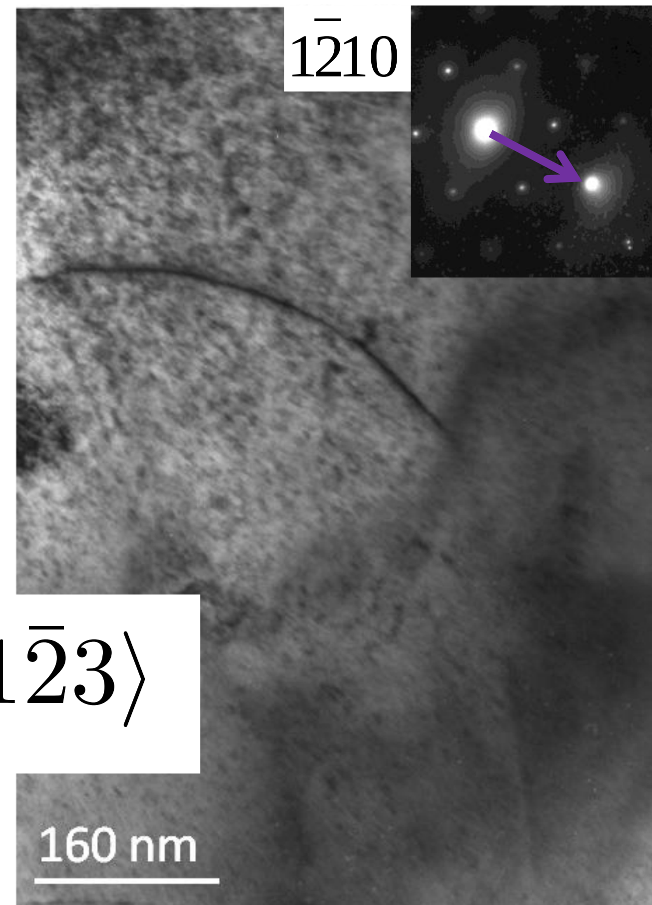
Non Basal Slip

$$g \cdot b \neq 0$$



$$g \cdot b = 0$$



$$b = \frac{a}{3}\langle 11\bar{2}3 \rangle$$

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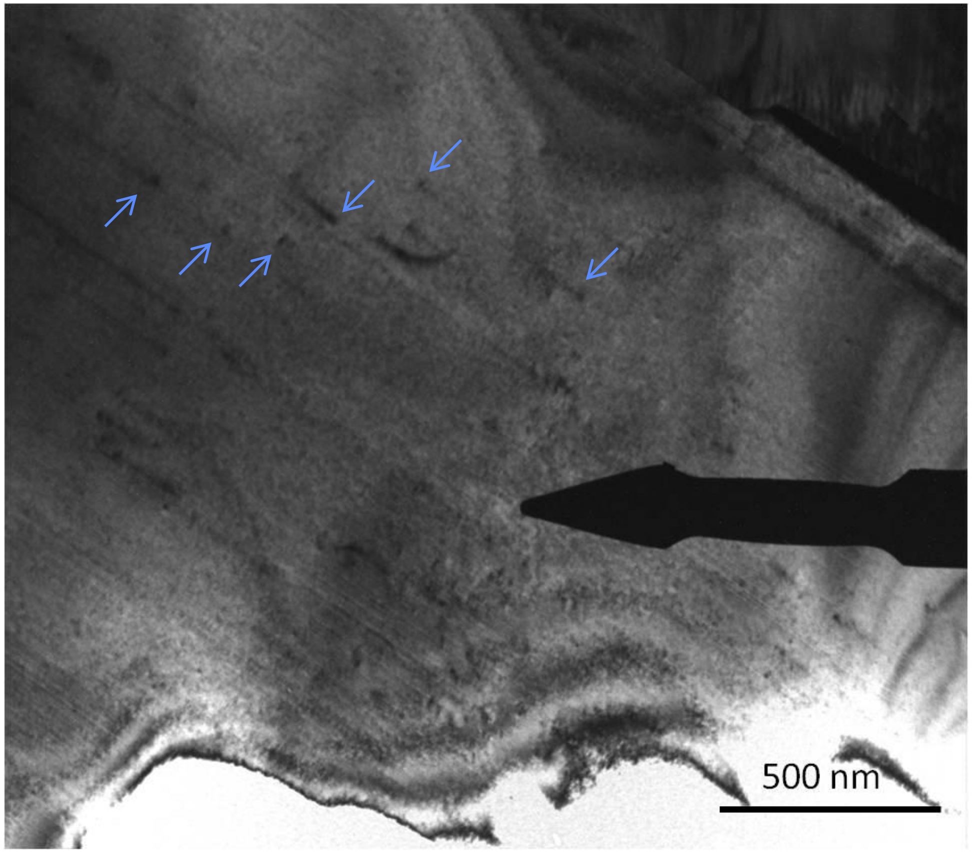
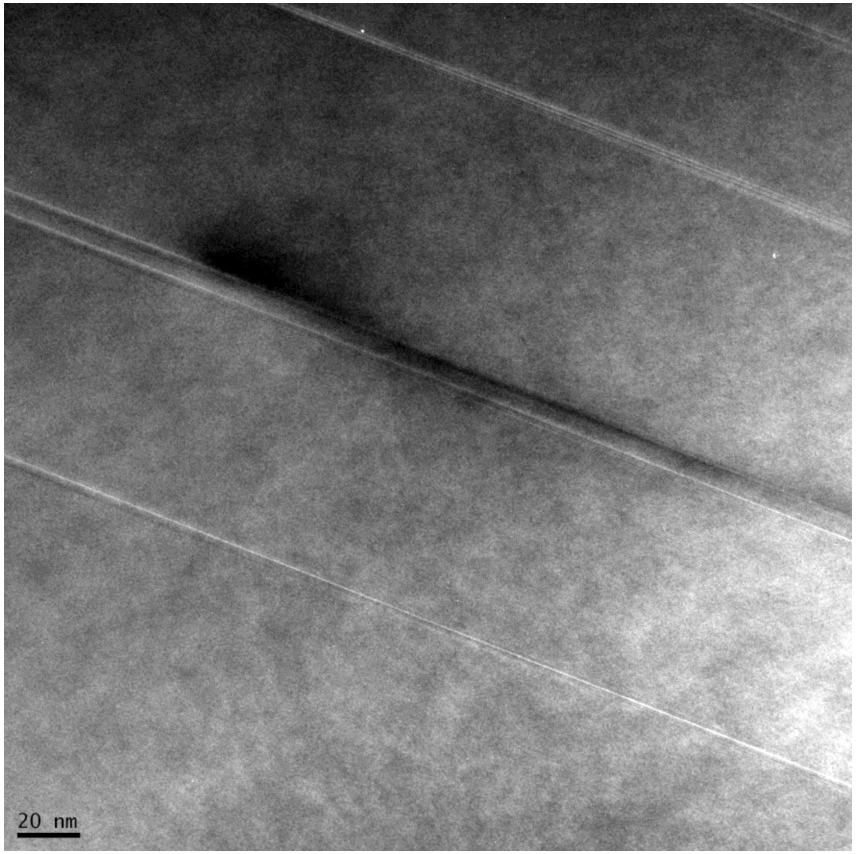
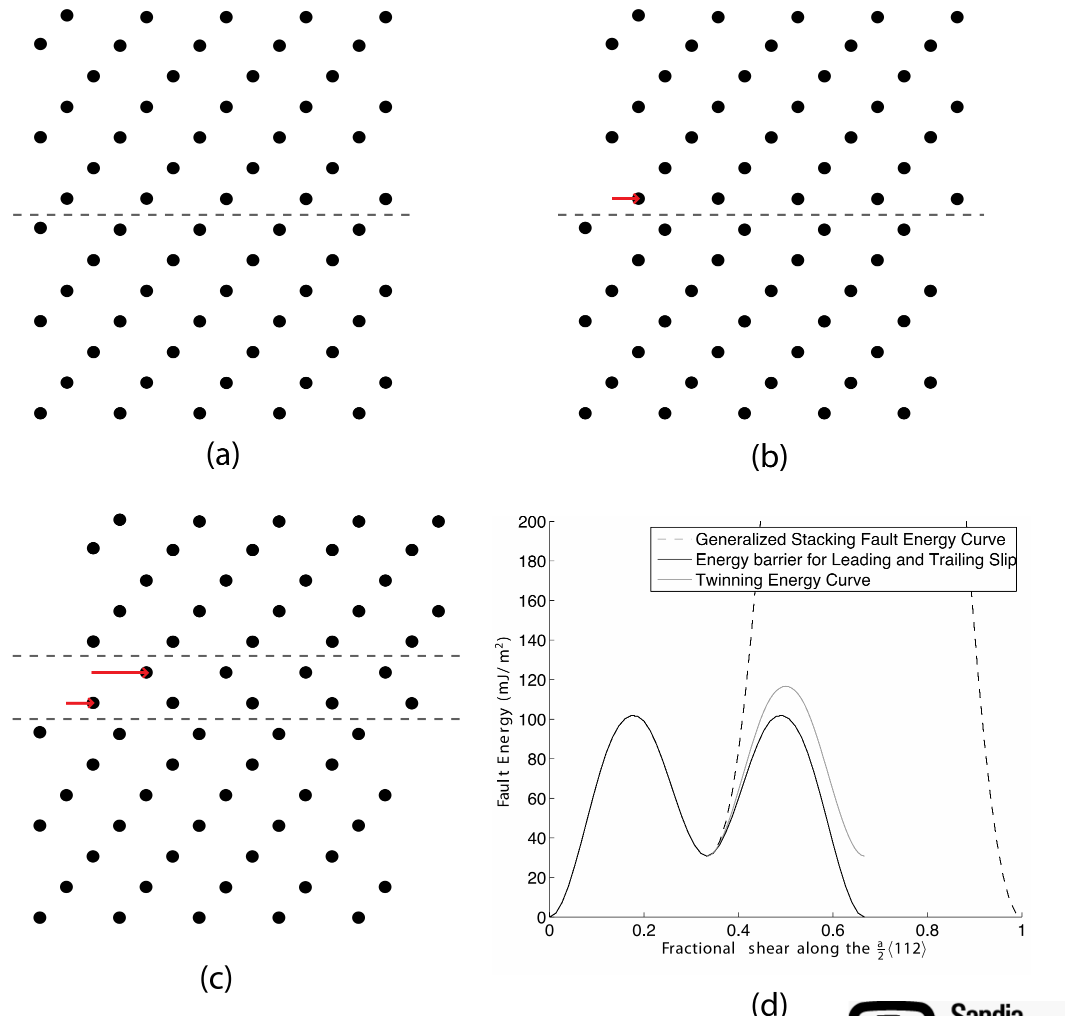
Basal Slip



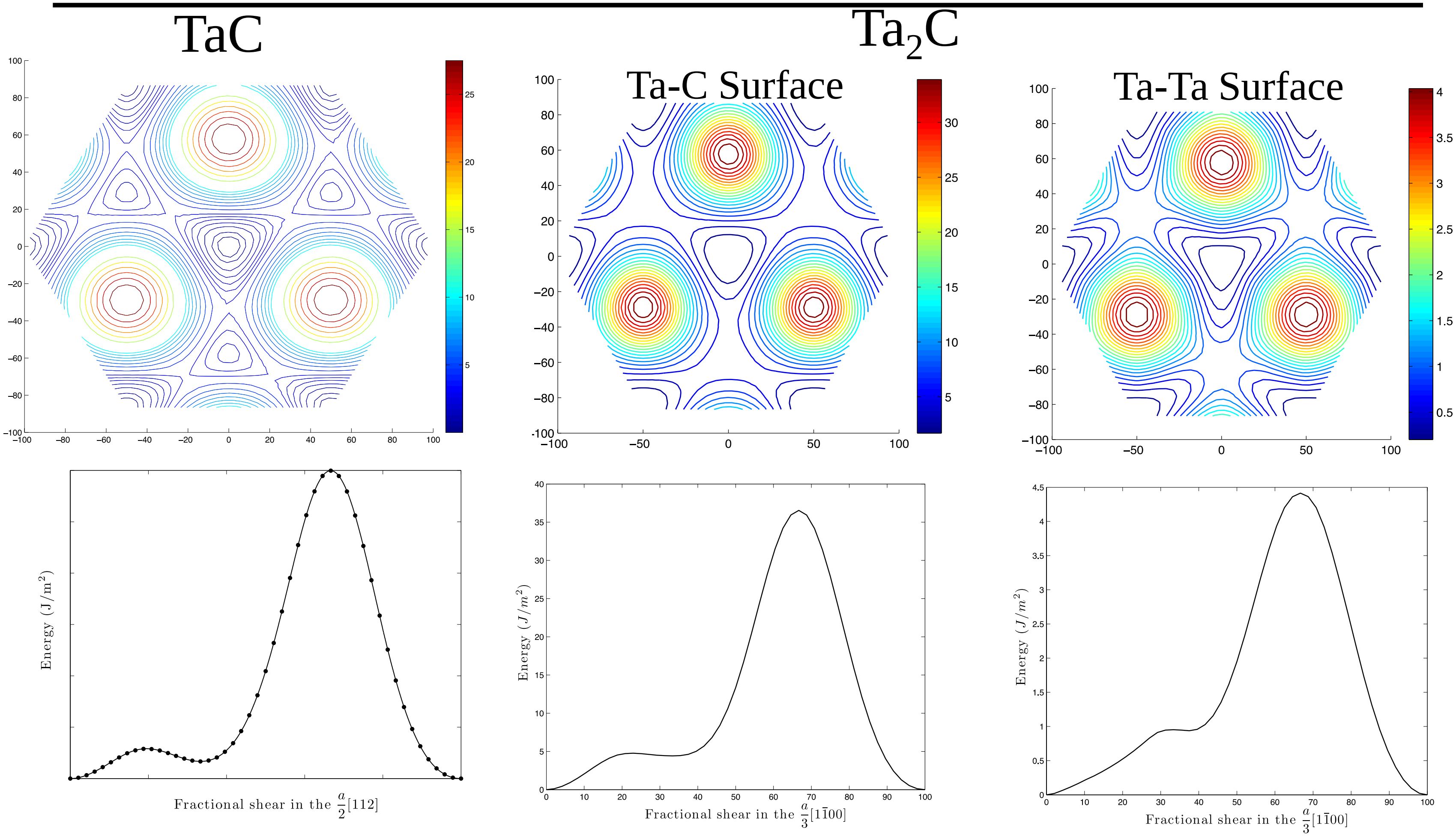


Generalized Stacking Faults

- Start with the energy of a perfect crystal (a).
- Cut a plane and slide the crystal by an aribtrary amount x (b).
- The GSF curve represents the energy difference between the perfect registry and the faulted structure (d).



Slip in TaC versus Ta_2C



Slip between the closed-packed planes in Ta2C (Ta-Ta) is easier than that of closed packed planes in TaC.

GSF Curves in Ta2C

Slip Plane	Slip Direction	Bonding	Maxima (J/m^2)	Ideal Strength (GPa)
{0001}	<01-10>	Ta-Ta	0.95	6.7
{0001}	<01-10>	Ta-C	4.48	59
{0001}	<11-20>	Ta-Ta	1.89	63
{0001}	<11-20>	Ta-C	12.5	130
{10-10}	<-12-10>	Ta-Ta	4.5	40
{10-10}	<-12-10>	Ta-C	7.9	51
{10-10}	<0001>	Ta-Ta	16.8	160
{10-10}	<0001>	Ta-C	7.8	120
{10-11}	<-12-10>	Ta-Ta	3.2	63
{10-11}	<-12-10>	Ta-C	7.5	81
{10-1-1}	<-12-10>	Ta-Ta	11.9	120
{10-1-1}	<-12-10>	Ta-C	8.0	81
{10-11}	<-2113>	Ta-Ta	3.1	27
{10-11}	<-2113>	Ta-C	4.9	54
{10-1-1}	<-2113>	Ta-Ta	76	750
{10-1-1}	<-2113>	Ta-C	54	54

Most favorable slip system.

GSF curves show that the most favorable slip systems agree with experimental observations <01-10>{0001} and <-2113>{10-11}

Second most favorable slip system.

Slip is generally favored between Ta-Ta bonds

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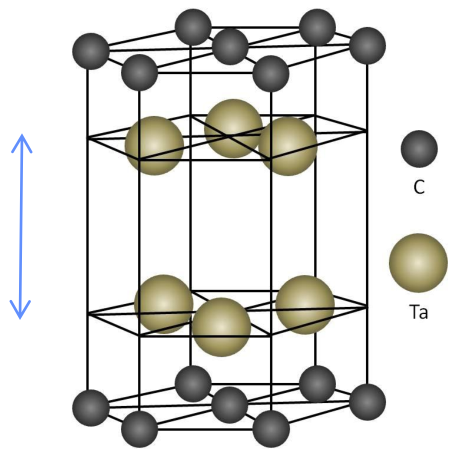
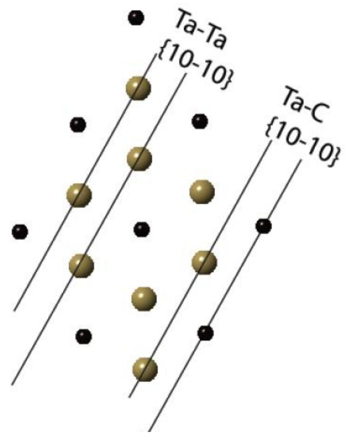
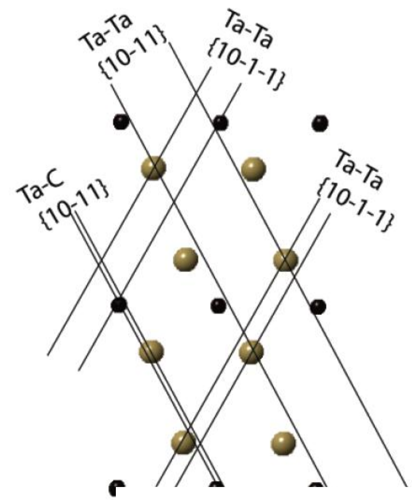
Inter-planar Spacing



Basal Planes



Prism Planes



Pyramidal Planes

The {0001} plane between Ta-Ta atoms has widest spacing

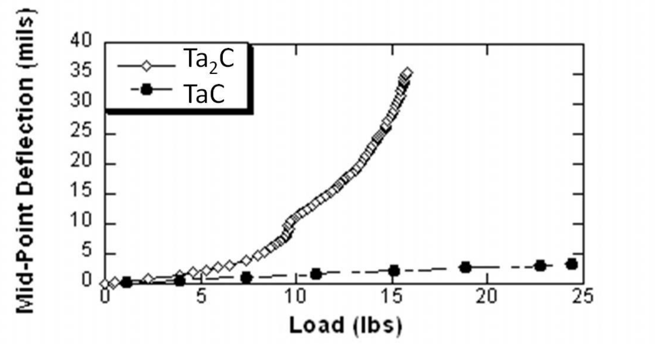
The {10-11} plane between Ta-Ta atoms has second widest spacing

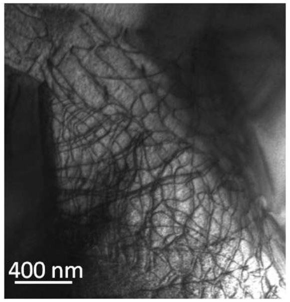
There is a strong positive correlation between GSF energies and inter-planar spacing. Inverse of the inter-planar spacing and max GSF energy are linearly related.

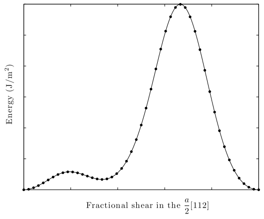
Slip in these mixed-metallic covalent bonded materials occurs between the most widely spaced planes.

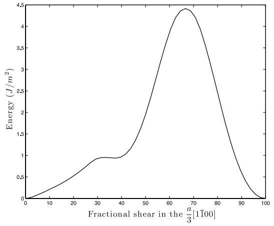
Conclusions

- Ta2C exhibits more plastic deformation than TaC at the same absolute temperature.
- Slip in Ta2C is dominated by basal slip, although pyramidal slip, <c+a>, dislocations contribute.
- Slip on the basal plane occurs between the Ta-Ta bonds
- GSF curves show that slip is easier in Ta2C on the basal plane than {111} slip in TaC.
- Slip occurs between the most widely spaced planes.









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