Interphase misorientation as a tool to study metamorphic and magmatic processes



Interphase Boundaries

Separates two different phases which may have different composition, crystal structure and/or lattice parameters

- Coherent interface → two crystals match perfectly at the interface plane (small lattice mismatch can be accommodated by elastic strain in the adjacent crystals)
- Semi-coherent interface → lattice mismatch is accommodated by periodic array of misfit dislocations
- Incoherent interface → disordered atomic structure of the interface







Incoherent







Coherent

Semicoherent

However...

- Geometry of interphase boundaries has received much less attention than grain boundaries in monomineralic aggregates
- Studies of metamorphic reactions have shown that nucleation and growth of new phases can be controlled by the crystallography of parent mineral
- Important to understand mineral reactions
- Interphase boundaries may influence interface diffusion (metamorphic processes) and rheology (e.g. phase mixing – deformation processes









relation 1 (100)_{Olivine} || (001)_{Antigorite} [001]_{Olivine} || [010]_{Antigorite} relation 2 (010)_{Olivine} || (001)_{Antigorite} [001]_{Olivine} || [010]_{Antigorite}

Boudier et al. 2010 – Journal of Petrology

ETHzürich Can we extrapolate these observations to larger scales?







McNamara et al. 2012 - JSG

To study the phase transformation between phase A and phase B

•We calculated the misorientation function (MDF) along grain boundaries between phase A and phase B;

• The MDF can be plotted as specific misorientation angles sections showing misorientation axes distribution in crystallographic coordinates;

•The MDF can be represented by misorientation angle histograms for all axes;

•Misorientation axes and angles corresponds to relations such as (100)pA || (001)pB & [001]pA || [010]pB in Burgers vector notation

•Those relations are geometrical and do not imply in a specific mechanism







Interphase misorientations - complications

- The distribution's fundamental region requires an entire upper hemisphere due to the combination of the orthorhombic symmetry of olivine and the monoclinic symmetry of antigorite.
- In addition, there is the constraint that grain 1 cannot be exchanged with grain 2 because they are clearly different physical entities.
- Therefore, there is no exchange symmetry across a phase boundary



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EXAMPLE 1 – olivine \rightarrow antigorite







Olivine – Antigorite

• Olivine to Serpentine (+ Brucite): $2Mg_2SiO_4 + 3H_2O = Mg_3Si_2O_5(OH)_4 + Mg(OH)_2$











Olivine-antigorite schist from Val Malenco





Morales et al. 2018 (Tectonophysics)



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Olivine-Antigorite misorientation angles for correlated, uncorrelated and uniform distributions



Interphase misorientation plots and maps

EBSD map of Section XY of olivine-antigorite boundaries with Burger relation No.4









Morales et al. 2018 (Tectonophysics)

Observed interphase relationships



EXAMPLE 2 – calcite-aragonite







Calcite-aragonite

- Heterogenenous nucleation and topotactic growth
- Metastable aragonite-rich mylonites can be found in areas that experienced high P-low T metamorphism (bluschists)
- Orientation relations described in the literature
- (11-20)_{cal} || [100]_{ar}
- [0001]_{cal} || [110]_{ar}
- Results presented here from hydrostatic experiment in a Griggs apparatus operating at









```
Cal2Ara No1 = orientation('map',...
 Miller(1,1,-2,0,ebsd('calcite').CS,'hkl'),Miller(1,0,0,ebsd('aragonite').CS,'hkl'),...
 Miller(0,0,0,1,ebsd('calcite').CS,'uvw'),Miller(0,1,1,ebsd('aragonite').CS,'uvw'))
õ
% check angles between hkl and uvw of parent and daughter to be 90 degrees
angle hkl uvw parent = angle(Miller(1,1,-2,0,ebsd('calcite').CS,'hkl'),...
                             Miller(0,0,0,1,ebsd('calcite').CS,'uvw'))/degree
angle hkl uvw daughter = angle(Miller(1,0,0,ebsd('aragonite').CS,'hkl')...
                              ,Miller(0,1,1,ebsd('aragonite').CS,'uvw'))/degree
% axis vector3d
axis No1 = vector3d(axis(Cal2Ara_No1))
% axis Aragonite
axis No1 Ara = axis(Cal2Ara No1)
% axis Calcite
axis No1 Cal = Miller(axis No1,ebsd('calcite').CS,'hkl')
% rotation angle
angle No1 = angle(Cal2Ara No1)/degree
% Euler angles
f1Ff2 No1 = Euler(Cal2Ara No1)/degree
% Olivine reference orientation Euler (0,0,0)
ori cal = orientation('Euler',0,0,0,ebsd('calcite').CS)
% Calculate all Daughter (Aragonite) variants
% by using all crystalloraphically equivalent orientations
% of Parent (Calcite)
ori Ara No1 = symmetrise(ori cal) * inv(Cal2Ara_No1)
```



Calcite pole figures

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Aragonite pole figures



Uniform MDF calcite-aragonite



Uniform MDF axis distribution



Correlated MDF – calcite-aragonite











Search for boundaries with specific angles

```
% N.B. With this method you select using uniquely the misorientation angle
       so if you have several different misorienation axes in a given
8
       angle interval they will be added together
8
% minimum:interval:maximum with interval = 5,10,15... etc try several
gb_m_axis_cor = axis(gB c a mis.project2FundamentalRegion);
gb m angle cor = angle(gB c a mis.project2FundamentalRegion)./ degree;
min angle = 10;
interval angle = 10;
maximum angle = 120;
[segments per interval, interval id] = histc(gb m angle cor, min angle: interval angle: maximum angle);
x bar=min angle:interval angle:maximum angle;
width=1;
clear percent boundary length n percent angle scale;
percent boundary length = zeros(length(segments per interval));
% total boundary length
total boundary length = sum(gB c a.seqLength);
% total number
total number = sum(segments per interval);
8
for i=1:length(segments per interval)-1;
% calculate boundary length in map units
boundary length = sum(gB c a(interval id==i).segLength);
% Percent boundary length
percent boundary length(i,1) = 100 * boundary length / total boundary length;
% Percent number
n percent(i,1) = 100 * segments per interval(i) / total_number;
    fprintf(' %3i %3i %s %3i %17.2f %12.2f %17.2f %12.2f \n',...
      i, x bar(i), '-
', x bar(i+1), boundary length, percent boundary length(i), segments per interval(i), n percent(i))
  angle scale(i, 1) = x bar(i);
end
```

%% Create search structure for boundary lengths per misorientation angle interval

Boundaries calcite-aragonite – mis=30-70°

```
plot(ebsd)
hold on
plot(grains('c').boundary,'linecolor','k','li
newidth',1)
plot(grains('a').boundary,'linecolor','k','li
newidth',1)
plot(gB c a(interval id==2), 'linecolor', 'r', '
linewidth',2,'displayName','20-30^\circ
8%', 'fiqSize', 'large')
plot(gB c a(interval id==3), 'linecolor', 'm', '
linewidth',2,'displayName','30-40^\circ
12%', 'figSize', 'large')
plot(gB c a(interval id==4), 'linecolor', 'c', '
linewidth',2,'displayName','40-50^\circ
14%', 'figSize', 'large')
plot(gB c a(interval id==5), 'linecolor', 'k', '
linewidth',2,'displayName','50-60^\circ
15%', 'figSize', 'large')
hold off
```





EXAMPLE 3 – gabbro from Atlantis Bank







What is the Atlantis Bank?







- Undersea mountain, named after the lost city of Atlantis;
- Middle of the ultra-slow spreading southwest Indian Ridge, southwest of Madagascar
- About 700 m below the sea level, approximately 1000 m height
- Result from the uplift along the Atlantis II transform faults, one of the biggest faults seen on Earth
- See presentation from Maël Allard this afternoon

"Squeezed melt" microstructures











Sample 118-56R - oxide-rich gabbro



Pole figures – plagioclase, olivine and ilmenite



Plagioclase pole figures



Ilmenite pole figures



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Interphase misorientation plagioclase \rightarrow olivine









Plagioclase - Olivine interphase boundaries









Plagioclase - Ilmenite interphase boundaries

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Interphase misorientation plagioclase →ilmenite

- Interphase boundary misorientation in EBSD maps is powerful method to understand orientation relationships between different phases in a statistically representative way;
- One can study the orientation relationships between two different phases whose orientation relationship is known, and in principle calculate other possible orientation relationships
- The advantage of this approach is that one can explore possible orientation relationships between any phase present in the map. Most of them won't show anything meaningful, but some pairs may show potential relationships
- The processes of course that lead to those are another business
- From this approach, one can precisely mark the interphase boundaries of interest, than bring the sample to the FIB, make TEM lamellae in the exact phase boundary you want to study (not "shooting in the dark")





