Self-adaptive and self-healing nanocomposite tribocoatings
Cao, Huatang

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Appendix 1 MATLAB script for calculations of wear volume

To measure the surface topography of the wear track, a µSurf Nanofocus confocal microscope is used. Based on the 3D confocal images of the wear track and assuming the polished surface is flat, a Matlab code in MK-RuG group (created by Dr. Jintao Sheng) is used to calculate the wear volume of the nanocomposite coating after wear. From each wear track, four images (north, east, south and west sides) were taken to calculate the average volume, with each of 727 × 705 µm size captured by using the camera 20x (the wear track width is normally < 200 µm, less than one-thirds the image size). The code defines two shoulders at the two sides of the wear track (flat intact coating parts), and then reconstructs the original surface by interpolating a flat surface between the shoulders. The wear volume is calculated by subtracting the wear track from the interpolated flat surface, thereby the wear rates are estimated.

% for track width less than 600 um, level surface with four corner areas.
% 1st step input parameters
radius=input('please input the radius of the wear track:');
direc=input('please input number of wear track direction (1=east,2=west, 3=north, 4=south):');
plan1minx=input('please input approximate min x of left or bottom plan area1:'); plan1minx =round(plan1minx *512/727);
plan1maxx=input('please input approximate max x of plan area1:'); plan1maxx =round(plan1maxx *512/727);
plan1miny=input('please input approximate min y of plan area1:'); plan1miny =round(plan1miny *512/727);
plan1maxy=input('please input approximate max y of plan area1:'); plan1maxy =round(plan1maxy *512/727);
plan2minx=input('please input approximate min x of plan area2 (two plans should be symmetric):'); plan2minx =round(plan2minx *512/727);
plan2maxx=input('please input approximate max x of plan area2:'); plan2maxx =round(plan2maxx *512/727);
plan2miny=input('please input approximate min y of plan area2:'); plan2miny =round(plan2miny *512/727);
plan2maxy=input('please input approximate max y of plan area2:'); plan2maxy =round(plan2maxy *512/727);
trackmin=input('please input approximate min of track:'); trackmin =round(trackmin *512/715);
trackmax=input('please input approximate max of track:'); trackmax =round(trackmax *512/715);
% 1st step calculate average plan height
h1=0; c1=0; h2=0; c2=0; h=0; diff=0;
for i= plan1minx:1: plan1maxx;
    for j= plan1miny:1: plan1maxy;
        h1=h1+data(512*(j-1)+i,3); c1=c1+1;
    end;
end;
for i= plan2minx:1: plan2maxx;
    for j= plan2miny:1: plan2maxy;
        h2=h2+data(512*(j-1)+i,3); c2=c2+1;
    end;
end;
h=(h1/c1+h2/c2)/2;
diff=h1/c1-h2/c2;

%2nd leveling
distplan=0; step=0;
if direc<=2;
    distplan=abs(plan2minx-plan1minx); step=diff/distplan;
for i=1:512;
    inc=0;
    for j=1:512;
        inc=(i-1)*step; data(512*(j-1)+i,3)=data(512*(j-1)+i,3)+inc;
    end;
end;
h1=0; c1=0; h2=0; c2=0;
for i= plan1minx:1: plan1maxx;
    for j= plan1miny:1: (plan1miny+20);
        h1=h1+data(512*(j-1)+i,3); c1=c1+1;
    end;
end;
for i= plan1minx:1: plan1maxx;
    for j= (plan1maxy-20):1: plan1maxy;
        h2=h2+data(512*(j-1)+i,3); c2=c2+1;
    end;
end;
diff2=0;
diff2=h1/c1-h2/c2;
distplan=abs(plan1maxy-plan1miny-20); step=diff2/distplan;
for i=1:512;
    inc=0;
    for j=1:512;
        inc=(j-1)*step; data(512*(j-1)+i,3)=data(512*(j-1)+i,3)+inc;
    end;
end;
elseif direc>2;
    distplan=abs(plan2miny-plan1miny); step=diff/distplan;
for i=1:512;
    inc=0;
    for j=1:512;
        inc=(j-1)*step; data(512*(j-1)+i,3)=data(512*(j-1)+i,3)+inc;
    end;
end;

h1=0; c1=0; h2=0; c2=0;
for i= plan1minx:1: (plan1minx+20);
    for j= plan1miny:1: plan1maxy;
        h1=h1+data(512*(j-1)+i,3); c1=c1+1;
    end;
end;

for i= (plan1maxx-20):1: plan1maxx;
    for j= plan1miny:1: plan1maxy;
        h2=h2+data(512*(j-1)+i,3); c2=c2+1;
    end;
end;

diff2=0;
diff2=h1/c1-h2/c2;
distplan=abs(plan1maxx-plan1minx-20);step=diff2/distplan;
for i=1:512;
    inc=0;
    for j=1:512;
        inc=(i-1)*step; data(512*(j-1)+i,3)=data(512*(j-1)+i,3)+inc;
    end;
end;
end;

% 3rd step retake the plan height
h1=0; c1=0; h2=0;c2=0;h=0;
for i= plan1minx:1: plan1maxx;
    for j= plan1miny:1: plan1maxy;
        h1=h1+data(512*(j-1)+i,3); c1=c1+1;
    end;
end;

for i= plan2minx:1: plan2maxx;
    for j= plan2miny:1: plan2maxy;
        h2=h2+data(512*(j-1)+i,3); c2=c2+1;
    end;
end;
h=(h1/c1+h2/c2)/2;

% 4th step cutoff the higher points
for i=1:512;
    for j=1:512;
        if data(512*(j-1)+i,3)-h>1;
data(512*(j-1)+i,3)=(data(512*(j-1)+i,3)-h)/5+h;
end;
end;
end;

% 5th step calculate the wear volume
dV=0; dA=0; dZ=0;
if direc<=2;
for i=1:512;
    dV=dV+dA*1.377; % total volume change equation
    dA=0;dZ=0; % set variable-- area change in one x-parallel line, height change per x point;
    for j= trackmin:1:trackmax; % x-min to x-max
        dZ=data(512*(i-1)+j,3)-h; % height change per x
        if dZ<1; % cutoff the debris in the wear track >1?m
            dA=dA+dZ*1.42; % area change in one y line
            c=c+1;
        end;
    end; % end of j loop
end; % end of i loop
mV=dV*2*pi*1000*radius/732;
mV
elseif direc>2;
for i= trackmin:1:trackmax;
    dV=dV+dA*1.377; % total volume change equation
    dA=0;dZ=0; % set variable-- area change in one x-parallel line, height change per x point;
    for j= 1:512; % x-min to x-max
        dZ=data(512*(i-1)+j,3)-h; % height change per x
        if dZ<1;
            dA=dA+dZ*1.42; % area change in one y line
            c=c+1;
        end;
    end; % end of j loop
end; % end of i loop
mV=dV*2*pi*1000*radius/710;
mV % the volume of the calculated wear track
end;
Figure A2.1 Cross-section of graded microstructure showing the tribofilm formed on the wear track after FIB milling.
Figure A2.2 Well-aligned $WS_2$ platelets along the wear track adjacent to the bulk coating with a sandwiched $WO_3$ layer.

Figure A2.3 Random distribution of dense $WS_2$ platelets in the middle part of the tribofilm.
Appendix 3 for Chapter 6

**Figure A3.1** (a, b) images with light microscopy of a wear track on the notched WS$_2$/a-C coating after sliding (small crack width: 2-5 µm); (c) Raman spectra of different areas as indicated in (a, b); (d) stable ultralow coefficient of friction with the inset showing a short running-in period, indicating no influence of the pre-notch on the triboperformance.
Figure A3.2 HR-TEM micrographs showing a panoramic cross-section of the healed notch (FIB-cut at the central part of wear track in Figure A3.1b): (a) overview of the self-healed notch with the marked box for higher magnification observation; (b-g) HR-TEM images showing WS$_2$ platelets re-orientated parallel to the local surface of the pre-notch; (h) HR-TEM image showing well aligned WS$_2$ platelets in the surface of the healed part parallel to the sliding direction; (i) HR-TEM image showing densified but randomly orientated WS$_2$ platelets in the central of the healed part.
Figure A3.3 (a) Stitched HR-TEM micrographs revealing reorientated WS$_2$ platelets along the curving interface at the bottom of the notch; (b) HR-TEM image at the notch interface distinguishing well aligned WS$_2$ (002) platelets in the healed notch from random ones in the raw coating; (c) HR-TEM image of the enriched and elongated WS$_2$ platelets near the interface. The dashed line indicates the tortuous interface of the healed notch/coating.
Figure A3.4. Corresponding selected area electron diffraction (SAED) patterns of circled areas 1-4 in Figure A3.2a: (a) top protective Pt; (3) Ga ion damaged gradient area from Pt to tribofilm with weak ring of WS$_2$; (c) the tribofilm filled into the cracked valley confirming both WS$_2$ and WO$_3$; (d) pristine coating showing mainly amorphous WS$_2$. Note (1) Pt JCPDS No. 04-0802; WS$_2$ JCPDS No. 08-0237; WO$_3$ JCPDS No. 43-1035 and (2) 10Z (Z=0, 1, 2,...stacking planes).
Figure A3.5 (a) low-magnified cross-section TEM image of the top part of the tribofilm filled into the notched damage; (b) HR-TEM image showing perfectly aligned WS$_2$ (002) platelets straightly parallel to the ball sliding direction (e.g. the coating surface). Note at the top part some materials are irradiated by FIB ion.