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################################################ surface_elasticity.sh begins here
# This is a sample LAMMPS script for calculating surface properties of Cu(100) surface.
# To calculate surface properties of other materials, lattice, create_box/atoms and potential should be changed in the following.

variable name string "Cu"
variable direction string "100"

units metal
boundary p p s

lattice fcc 3.615 origin 0 0 0 orient x 0 1 0 orient y 0 0 1 orient z 1 0 0                # for (100) surface

variable a equal 2
variable b equal 10
region                  mybox block -$a $a -$a $a -$b $b

create_box              1 mybox
create_atoms            1 region mybox

pair_style              eam
pair_coeff              * * ${name}_u3.eam


mass * 0.1

neigh_modify every 1 delay 0 check yes
minimize            1e-12 1e-14 10000 100000      # relaxed surface at zero strain as initial state

write_restart ./dump/dump.restart.${name}

variable strain_direction equal "1212"
############################################################

variable max_strain equal 0.01       # change from -${max_strain} ~ ${max_strain}
variable n equal 41          # iteration numbers - only run n times of simulation
variable i loop $n

label loopa
variable strain equal (2*($i-1)/($n-1)-1)*${max_strain}

pair_style              eam
pair_coeff              * * ${name}_u3.eam
```

```
compute pe_atom all pe/atom

# apply tensile strain
variable strain_scale equal ${strain}+1
# change_box all x scale ${strain_scale} remap units box
#change_box all x scale ${strain_scale} y scale ${strain_scale}      remap units box

# apply shear strain
variable tmp equal ly
variable ly0 equal ${tmp}
variable delta equal ${ly0}*${strain}
change_box all triclinic
change_box all xy delta ${delta} remap units box

# apply shear strain
# variable tmp equal lz
# variable lz0 equal ${tmp}
# variable delta equal ${lz0}*${strain}
# change_box all triclinic
# change_box all xz delta ${delta} remap units box

dump                    1                    all                    custom
1000000  ./dump/dump.${name}${direction}.strain_${strain_direction}_max_${max_strain}_i_$i.l
mp id type x y z c_pe_atom                  # only the final snapshot is useful
dump_modify 1 format float %20.15g

neigh_modify every 1 delay 0 check yes
minimize          1e-12 1e-14 10000 100000

undump 1

clear
read_restart ./dump/dump.restart.${name}

next i
jump surface_elasticity.sh loopa
################################################ surface_elasticity.sh ends here

################################################ surface_elasticity.m begins here
% This is a sample LAMMPS script for calculating surface properties of Cu(100) surface.

clear;close all;clc;

surface_direction='100';
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```
strain_direction='1212';
max_strain=0.01;
n=41;

filename='./dump/dump.Cu';

% get initial surface
file=[filename surface_direction '.strain_' strain_direction '_max_' num2str(max_strain) '_i_'
num2str((n+1)/2) '.lmp'];
dump=readdump_one(file,-1,6);
xbound=dump.x_bound;
ybound=dump.y_bound;
zbound=dump.z_bound;
S0=(xbound(2)-xbound(1))*(ybound(2)-ybound(1));
data=dump.atom_data;
Z=data(:,5);
Pe=data(:,6);

[C,I]=min(abs(Z));
A0=Pe(I);
E0=(sum(Pe)-A0*length(Pe))/2/S0*1.6022*10^(-19)/10^(-20);    % J/m^2

strain=zeros(n,1);
energy=zeros(n,1);
for i=1:n
    strain(i)=(2*(i-1)/(n-1)-1)*max_strain;
    file=[filename surface_direction '.strain_' strain_direction '_max_' num2str(max_strain) '_i_'
num2str(i) '.lmp'];
    dump=readdump_one(file,-1,6);
    data=dump.atom_data;
    Pe=data(:,6);
    Z=data(:,5);

    [C,I]=min(abs(Z));
    A0=Pe(I);
    energy(i)=(sum(Pe)-A0*length(Pe))/2/S0*1.6022*10^(-19)/10^(-20);    % J/m^2
end

[b,bint,r,rint,stats]=regress(energy,[ones(n,1) strain 0.5*(strain.*strain)])
% b(1)=s0
% if it's 1111/1212 dir, then b(2)=s11/s12 (usually s12=0) and b(3)=s1111/s1212
% if it's 1122 dir, then b(2)=s11+s22 (it can be used to check b(2)=s11+s22 or b(2)=2s11 if s11=s22)
%                       and b(3)=s1122+s2211+s1111+s1122 (usually s1122=s2211)
%                        so s1122=(b(3)-s1111-s2222)/2 or s1122=b(3)/2-s1111 if s1111=s2222
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```
plot(strain,energy,strain,energy,'*')
xlabel('strain, \epsilon_{12}');ylabel('surface energy, \Gamma (J/m^2)')
############################################### surface_elasticity.m ends here
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