

Main codes for matrix generating and fitting:

Find peak:

```
subplot(3, 1, [1 2])
PH = 150;
minDistance = 0.1;
findpeaks(I, Po, 'MinPeakHeight', PH, 'MinPeakDistance', minDistance);
[pks, locs]=findpeaks(I, Po, 'MinPeakHeight', PH, 'MinPeakDistance',
minDistance);
size(pks,1)
```

Add more peak:

```
inputpk = input('Input more peaks?', 's');
switch inputpk
    case {'Y', 'y'};
        nwpkslocation = input('Input peak locations:');
        nwpksintensity = input('Input peak intensities:');
        npks = [pks;nwpksintensity'];
        nlocs = [locs;nwpkslocation'];
        NmPeaks = size(npks, 1)
    case {'N', 'n'};
        npks = pks;
        nlocs = locs;
end
subplot(3, 1, [1,2]);
hold on;
stem(nlocs, npks)
hold off;

pkmodify = input('Modify input pks? ', 's')
switch pkmodify
    case {'y', 'Y'};
        display(nwpkslocation);
        modifypkslocation = input('Input new peak locations: ');
        display(nwpksintensity);
        modifypksintensity = input ('Input new peak intensities: ');
        npks = [pks;modifypksintensity'];
        nlocs = [locs;modifypkslocation'];
        NmPeaks = size(npks, 1)
    case {'N', 'n'};
        display('No peaks modified')
end
stem(nlocs, npks)
xlim([left_base, right_base]);
```

Matrix Generator

```
M.PeakWidth = ones(size(nlocs,1),1);
M.PeakLocation = nlocs;
M.PeakHeight = npks;
GauLorenF = 'u*c*exp(-(x-b)/a).^2+(1-u)*c*(a.^2*(a.^2+(x-b).^2).^-1)+z+';
GLM.GauLorenf =strseq ('lf', [1:1:size(M.PeakHeight,1)]) ;
for i = 1:size(M.PeakHeight,1);
    GLM.GauLorenf(i)= {strrep(GauLorenF, 'a', sprintf('a%02d',i))};
end
for j = 1:size(M.PeakHeight,1);
    GLM.GauLorenf(j)= strrep(GLM.GauLorenf(j), 'b', sprintf('b%02d',j));
end
```

```

for k = 1:size(M.PeakHeight,1);
    GLM.GauLorenf(k)= strrep(GLM.GauLorenf(k),'c', sprintf('c%02d',k));
end

fit_functionp = cell2mat(GLM.GauLorenf');
fit_function = fit_functionp(1, 1:size(fit_functionp,2)-1);
GLft = fittype (fit_function);
ParM = [0 0 0];

Peak fitting
warning off backtrace
tic
T1 = table(0, 0, 0, 0, 'VariableNames', {'aw', 'ai',
'rsquare', 'NormalizedRMSE',});
CFitStruc = struct('FitStruc', [], 'aw', 0, 'ai', 0, 'rsquare',
0, 'NormalizedRMSE', 0 );
AveI = mean(I);
subplot(3, 1, [1, 2])
hold on
plot(Po, I)
grid on
xlim manual
xlim([left_base, right_base])

subplot(3, 1, 3)
grid on
xlim manual
xlim([left_base, right_base])
ylim([-AveI, AveI])

Z = zeros(10,10);
RR = zeros(10, 10);
i=0;
j=0;

for aw = 1:1:10
    i=i+1;
    for ai = 1:1:10
        j=j+1;
        [i, j]
        hold on
        [GL_ft, GLgof]=fit(Po,I,GLft, 'Lower', zeros(1,3*size(nlocs,1)+2),
'StartPoint', [(aw/10)*M.PeakWidth' M.PeakLocation'
(ai/10)*M.PeakHeight', 0, 0]);
        subplot(3, 1, [1, 2]);
        plot(GL_ft);
        drawnow
        pl.Color = [aw/10, 0, 0];
        xlim([left_base, right_base]);
        legend('off')

        Z(i, j) = GLgof.rmse/AveI;
        RR(i, j) = GLgof.rsquare;

        subplot(3, 1, 3)
        grid on

```

```

hold off
legend('off')
rdsp = plot(GL_ft,Po,I,'Residuals');
drawnow
axis manual
xlim([left_base, right_base]);
ylim([-AveI, AveI]);
rdsp(1,1).LineStyle = '-';
rdspaxis=gca;
rdspaxis.XLim =[left_base, right_base];
rdspaxis.YLim =[-AveI, AveI];
%legend('Residuals', 'Zero Line')

T1.aw(size(T1.aw,1)+1,:) = aw;
CFitStruc(size(T1.aw,1),:).aw = aw;
T1.ai(size(T1.aw,1),:) = ai;
CFitStruc(size(T1.aw,1),:).ai = ai;
T1.rsquare(size(T1.aw,1),:) = GLgof.rsquare;
CFitStruc(size(T1.aw,1),:).rsquare = GLgof.rsquare;
T1.NormalizedRMSE(size(T1.aw,1),:) = GLgof.rmse/AveI;
CFitStruc(size(T1.aw,1)).NormalizedRMSE = GLgof.rmse/AveI;
CFitStruc(size(T1.aw,1)).FitStruc = GL_ft;

end
j=0;
end
format short

eptime = toc;
%endt= [num2str((cputime-startt)/60), ' min']

format long
Run = strseq ('Run', [0:1:size(T1,1)-1]);
CFitStruct = struct2table(CFitStruc);
CFitStruct.Properties.RowNames = Run;
T1.Properties.RowNames = Run;
CFitStruct2 = sortrows(CFitStruct, 'NormalizedRMSE', 'ascend');
CFitStructSorted = table2struct(CFitStruct2);

figure
subplot(5,1,[1,2])
grid on
plot(Po, I, 'k--')
hold on;
plot(CFitStructSorted(2).FitStruc)
plot(CFitStructSorted(3).FitStruc)
plot(CFitStructSorted(4).FitStruc)
hold off
subplot(5,1,3)
grid on
rdsp3=plot(CFitStructSorted(2).FitStruc, Po, I, 'Residuals');
rdsp3(1,1).LineStyle = '-';
rdsp3paxis = gca;
rdsp3paxis.YLim=[-AveI, AveI];
rdsp3paxis.XLim =[left_base,right_base];

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```

        legend('Top1 Residuals', 'Zero Line')
subplot(5,1,4)
grid on
rdsp4= plot(CFitStructSorted(3).FitStruc, Po, I, 'Residuals');
rdsp4(1,1).LineStyle = '-';
    rdsp4axis = gca;
    rdsp4axis.YLim=[-AveI, AveI];
    rdsp4axis.XLim =[left_base,right_base];
    legend('Top2 Residuals', 'Zero Line')
subplot(5,1,5)
grid on
rdsp5=plot(CFitStructSorted(4).FitStruc, Po, I, 'Residuals');
rdsp5(1,1).LineStyle = '-';
    rdsp5axis = gca;
    rdsp5axis.YLim=[-AveI, AveI];
    rdsp5axis.XLim =[left_base,right_base];
    legend('Top3 Residuals', 'Zero Line')

SortT1 = sortrows(T1, 'NormalizedRMSE','ascend');
Top3Run = SortT1(1:4,:);

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```

endt = strcat(num2str(eptime/60), ' min')

```

Measurements

```

clf
clear a b c u z
tncoeff = zeros(4,3*size(nlocs,1)+2);
for n = 2:4
tncoeff(n,:) = coeffvalues(CFitStructSorted(n).FitStruc);
end

for m = 1:3
i=length(tncoeff(m+1,:));
j=(length(tncoeff(m+1,:))-2)/3;
a(m,:)=[tncoeff(m+1,1:j)];
b(m,:)=[tncoeff(m+1,j+1:i-j-1-1)];
c(m,:)=[tncoeff(m+1,i-j+1-1-1:i-2)];
u(m,:) = tncoeff(m+1,i-1);
z(m,:) = tncoeff(m+1,i);
end

x = linspace(left_base, right_base, 1000);
for l = 1:3
A =find_GLpeaks(a(l,:), b(l,:), c(l,:),u(l,:),z(l,:),x);
    if isempty(find(~A, 1)) == 1
        disp('non zero peak fit')
    elseif isempty(find(~A, 1)) == 0
        disp('zero peak fit in matrix A')
    end
    B(l,:) = sum(A,1);
    clf
    findbp=findobj(boxplot(A(:,3)));
    FWHMoutliers = findbp(7,1).YData;
    ModifiedFWHM(l,:) = B(l,3) - sum(FWHMoutliers);
end
hold off

```

```

while size(B,1)>1
fig = input('Which figure would be generated: fig1, fig2, fig3, or press q
end to quit scripts? ', 's');
switch fig
case 'fig1'
figure
subplot(3,1,[1, 2])
A1 =find_GLpeaks(a(1,:), b(1,:), c(1,:),u(1,:),z(1,:),x);
if isempty(find(~A1, 1)) == 1
disp('non zero peak fit')
elseif isempty(find(~A1, 1)) == 0
disp('zero peak fit in matrix A')
end
subplot(3,1,3)
grid on
rds=plot(CFitStructSorted(2).FitStruc, Po,I,'Residuals');
rds(1,1).LineStyle = '-';
rdsaxis = gca;
rdsaxis.YLim=[-AveI, AveI];
rdsaxis.XLim =[left_base,right_base];
legend('Residuals', 'Zero Line')
Tfig1 = table(B(1,3),ModifiedFWHM(1,:),
B(1,1)/B(1,3),AveI,'VariableNames',{'SumFWHM', 'ModifiedFWHM', 'IndexRatio',
'AveI'})
T2fig1 = table(u(1), z(1), 'VariableNames', {'u', 'z'})
T3fig1 = Top3Run(2,:);
hold on
subplot(3, 1, [1 2])
whitebg ([1 1 1])
xlim([left_base, right_base])
ylim([min(y),max(y)])
h1=plot(Po,I,'k-', 'MarkerSize', 1, 'LineWidth', 1);
h2=plot(CFitStructSorted(2).FitStruc,'m-.');
h2.LineWidth = 1;
legend([h1 h2], 'raw data', 'fitted curve')

tstr=strrep(strcat(picname(1,1:17),', Fit1'), '_', ' ');

title(tstr);

t1 = tstr;

case 'fig2'
figure
subplot(3,1,[1, 2])
A2 =find_GLpeaks(a(2,:), b(2,:), c(2,:),u(2,:),z(2,:),x);
if isempty(find(~A2, 1)) == 1
disp('non zero peak fit')
elseif isempty(find(~A2, 1)) == 0
disp('zero peak fit in matrix A')
end
subplot(3,1,3)
grid on
rds=plot(CFitStructSorted(3).FitStruc, Po,I,'Residuals');
rds(1,1).LineStyle = '-';
rdsaxis = gca;
rdsaxis.YLim=[-AveI, AveI];

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rdsaxis.XLim =[left_base,right_base];
legend('Residuals', 'Zero Line')
Tfig2 = table(B(2,3),ModifiedFWHM(2,:), B(2,1)/B(2,3), AveI,
'VariableNames',{'SumFWHM', 'ModifiedFWHM', 'IndexRatio', 'AveI'})
T2fig2 = table(u(2), z(2), 'VariableNames', {'u', 'z'})
T3fig2 = Top3Run(2,:)

hold on
subplot(3, 1, [1 2])
whitebg ([1 1 1])
xlim([left_base, right_base])
ylim([min(y),max(y)])
h1=plot(Po,I,'k-', 'MarkerSize', 1, 'LineWidth', 1);
h2=plot(CFitStructSorted(3).FitStruc,'m-.');
h2.LineWidth = 1;
legend([h1 h2], 'raw data', 'fitted curve')

tstr=strrep(strcat(picname(1,1:17),', Fit2'), '_', ' ');
title(tstr);
t2 = tstr;

case 'fig3'
figure
subplot(3,1,[1, 2])
A3 =find_GLpeaks(a(3,:), b(3,:), c(3,:),u(3,:),z(3,:),x);
if isempty(find(~A3, 1)) == 1
disp('non zero peak fit')
elseif isempty(find(~A3, 1)) == 0
disp('zero peak fit in matrix A')
end
subplot(3,1,3)
grid on
rds=plot(CFitStructSorted(4).FitStruc, Po,I,'Residuals');
rds(1,1).LineStyle = '-';
rdsaxis = gca;
rdsaxis.YLim=[-AveI, AveI];
rdsaxis.XLim =[left_base,right_base];
legend('Residuals', 'Zero Line')
Tfig3 = table(B(3,3),ModifiedFWHM(3,:),
B(3,1)/B(3,3),AveI, 'VariableNames', {'SumFWHM', 'ModifiedFWHM', 'IndexRatio',
'AveI'})
T2fig3 = table(u(3), z(3), 'VariableNames', {'u', 'z'})
T3fig3 = Top3Run(4,:)
hold on
subplot(3, 1, [1 2])
whitebg ([1 1 1])
xlim([left_base, right_base])
ylim([min(y),max(y)])
h1=plot(Po,I,'k-', 'MarkerSize', 1, 'LineWidth', 1);
h2=plot(CFitStructSorted(2).FitStruc,'m-.');
h2.LineWidth = 1;
legend([h1 h2], 'raw data', 'fitted curve')
tstr=strrep(strcat(picname(1,1:17),', Fit3'), '_', ' ');
title(tstr);
t3 = tstr;
case 'q'
break;
end
end

```

end