Relatório Final

Gerando redes cristalinas de fluorapatita e clorapatita usando dinâmica molecular

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Resumo de atividades:

O projeto propõe, como objetivo central, simular uma rede cristalina e apatita, isso mais tarde será útil para testar o modelo de reconstituição dos traços de fissão via "thermal annealing".

Até então, todos os outros modelos que quantificaram o processo de reconstituição dos traços de fissão nas redes cristalinas eram puramente estatísticos, i.e., não se preocupavam em explicar o processo físico por traz dessa reconstituição, simplesmente achavam uma modelagem que fitava bem os dados.

Primeiramente comecei estudando o modelo proposto por Gleadow et al em uma série de quatro artigos.

O primeiro deles faz uma descrição qualitativa do problema, levantando quais são os fatores dominantes para a reconstituição dos traços de fissão na rede cristalina e basicamente divide o processo em duas etapas.

O processo dominante para a reconstituição dos traços de fissão da rede é de longe a

temperatura.

Para pequenos graus de “thermal annealing” o processo dominante faz com que o tamanho l dos traços diminua gradualmente, com os traços perpendiculares ao eixo-c reduzindo mais rapidamente dos que o paralelo ao mesmo. Até que quando $l/lo < 0.65$ (onde lo é o tamanho do traço antes do aquecimento) o processo se torna mais intenso e os traços passam a se fragmentar em porções descontínuas. (2)

O segundo deles faz uma descrição quantitativa do problema, foi-se observado que se podia aplicar a lei de Arrhenius para criar modelos estatísticos dos “thermal annealing” de traços de fissão com temperatura constante, dentre eles os mais famosos são “The parallel Arrhenius plot” e “The Fanning Arrhenius plot”. (3)

O terceiro deles tenta agora atacar o problema de “thermal anneling” de traços de fissão com temperatura variável, assumindo, de maneira ad hoc, o chamado “principio do tempo equivalente”, que basicamente diz que a qualquer momento, um traço que foi aquecido a um certo grau se comporta durante o resto do aquecimento de uma forma que é independente das condições que causaram o aquecimento antes, mas que depende apenas do grau de aquecimento que ocorreu e as condições prevalecentes de temperatura e tempo. (4)

O quarto e último dos artigos utiliza o modelo descrito em (4) para descobrir a história térmica e a idade de um determinado mineral. (5)

Por fim, estudou-se o modelo de proposto por S. Guedes que tenta descrever um processo físico para a reconstituição dos traços, como pode ser visto em (1).

Após estudar os modelos, familiarizou-se um pouco com a linguagem de programação FORTRAN, pois a mesma seria necessária para o desenvolvimento do programa que geraria as nano apatitas.

Como o trabalho envolvia simulações, recomendou-se que o aluno lesse um pouco sobre a história da simulação computacional e que lesse sobre dinâmica molecular.

Dentre os algoritmos que o livro menciona, o mais usado, segundo o mesmo, é o Verlet. Por isso aluno achou pertinente, dentre todos os tópicos que abrangem dinâmica molecular, descrever quantitativamente ele. O método da uma solução numérica para equações do tipo (que incluem a segunda lei de Newton):

$$a*(d^2r(t)/dt^2) = f(r(t))$$

Sendo a uma constante. A idéia do método é expandir $r(t + \delta t)$, que seria a posição de um partícula após um passo δt, em uma série de Taylor:

$$r(t + \delta t) = r(t) + (dr(t)/dt)* \delta t + (d^2r(t)/dt^2)*(\delta t^2)/2 + (d^3r(t)/dt^3)*(\delta t^3)/6 + O(\delta t\text{^}4) \quad \text{eq.1}$$

Agora se expande r(t-δt) em uma série de Taylor:

$$r(t - \delta t) = r(t) - (dr(t)/dt)* \delta t + (d^2r(t)/dt^2)*(\delta t^2)/2 - (d^3r(t)/dt^3)*(\delta t^3)/6 + O(\delta t^4) \text{ eq.2}$$

Pode-se isolar r(t + δt) apenas em função de r(t - δt), r(t) e sua aceleração $d^2r(t)/dt^2$, em t, introduzindo um erro da ordem de O(δt^4):

$$r(t + \delta t) = 2*r(t) – r(t - \delta t) + (d^2r(t)/dt^2)*(\delta t^2) + O(\delta t^4)$$

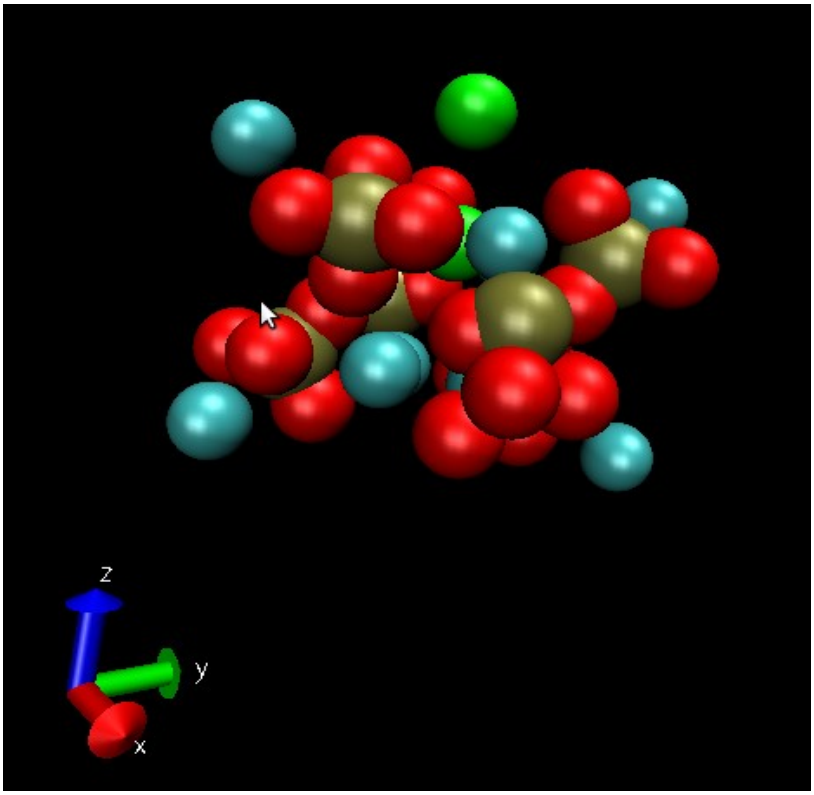
Onde $d^2r(t)/dt^2*(\delta t^2)$ é obtido diretamente de f(r(t))/a.

Pode-se também determinar a velocidade, útil para cálculos de energia cinética, v(t) = dr(t)/dt. Subtraindo a eq.2 da eq.1 e isolando v(t):

$$v(t) = (r(t + \delta t) – r(t – \delta t))/(2*\delta t) + O(\delta t^2)$$

Feito isso o aluno começou a elaborar a primeira parte programa que geraria um cristal de fluorapatita, após consultar o livro “Crystal structures”(6) para saber a posição de cada átomo da fluorapatita, gerou-se um programa em FORTRAN que sequenciava esses átomos de modo formar a rede cristalina, o output desses programa (a posição de cada átomo na rede) seria o CONFIG, um dos inputs do programa DL POLY 4.0, responsável para gerar o cristal.

Uma molécula de fluorapatita foi obtida usando o software VMD – Visual Molecular Dynamics. A figura se encontra abaixo:



Visualização da molécula de fluorapatita: os átomos vermelhos representão o oxigênio, os verdes o fluor, o dourado o fósforo e os azuis claro o cálcio.

O outro input necessário era a criação do arquivo CONTROL, que da informação sobre o tipo de ensemble usado, o tempo de cada interação moleculare e o número e alcance dessas interações.

Por último e mais complicado é a criação do FIELD, que dita o tipo de interação entre os átomos, o valor dos potenciais para a fluorapatita pode ser encontrado em (7), por ter muitos átomos não está sendo fácil acertar o FIELD e fazê-lo entrar em harmonia com os outros inputs.

O FIELD é um arquivo complexo, é nele que está contida a informação necessária para se descrever a interação entre os átomos . A molécula de fluorapatita tem 42 átomos e isso faz com que seja ligeiramente complicado dar os tipos de potenciais entre os átomos.

No nosso caso o alcance do potencial foi da ordem de 8 angstroms que é o equivalente a considerar apenas os átomos vizinhos, caso contrário ficaria muito complicado. Com essas aproximações ainda tivemos cerca de 600 potenciais, entre buck, shell e potenciais de três corpos. Como isso não é (e nem é possível) uma descrição exata

do problema para fazer a molécula se tornar estável (e portanto gerar a rede) é preciso que esses potenciais não façam a molécula colapsar, se eles forem demasiados ela vai ser comprimida e o programa DL_POLY 4 vai dar erro. Se eles forem de menos ela vai se expandir e novamente teremos um erro. Por isso, apesar dos arquivos terem sido criados, ainda há alguma correções a serem feitas para fazer a estrutura ficar estável.

Produção científica:

Código em FORTRAN 90 que gerou o CONFIG:

```
PROGRAM cellgen
!
!    Program to generate fluorapatite simulation cell of desired size
!    Written by Heitor do A. Jurkovich, Universidade Estadual de Campinas, Brazil
!    Reads fractional coordinates of 42 ions in the unit cell
!    Changes cell boundaries from (0., 1.) to (-0.5, 0.5)*cell
!
     IMPLICIT NONE
     REAL, DIMENSION(68):: xfr, yfr, zfr
     REAL :: alatt, blatt, clatt, tstep, cell1, cell5, cell9, zero
     REAL :: xstart, ystart, zstart, tottime
     INTEGER, DIMENSION(68) :: id
     INTEGER:: ncellx, ncelly, ncellz, levcfg, imcon, nstep
     INTEGER:: iatom, index, ix, iy, iz
     CHARACTER(LEN=8), DIMENSION(11) :: sym
     OPEN(1,file='apatite.in',status='old')
     DO index = 1, 68
     read (1,*) id(index), xfr(index), yfr(index), zfr(index)
     ENDDO
     READ(1,*) ncellx, ncelly, ncellz, levcfg, imcon, nstep, tottime
     READ(1,*) alatt, blatt, clatt, tstep
     CLOSE(1)
     iatom = 0
     cell1  = real(ncellx)*alatt
     cell5  = real(ncelly)*blatt
     cell9  = real(ncellz)*clatt
     zero   = 0.
     xstart = -0.5*cell1
     ystart = -0.5*cell5
     zstart = -0.5*cell9
     OPEN(2,file='CONFIG',status='new')
```

```
      WRITE(2, *) 'Apatite wil lattice parameters:', ncellx, ncelly, ncellz
      WRITE(2,'(3i10,2g20.10)') levcfg, imcon, nstep, tstep, tottime
      IF(imcon.gt.0) THEN
         WRITE(2,'(3f20.10)') cell1, zero,  zero,&
                              zero,  cell5, zero,&
                              zero,  zero,  cell9
      ENDIF
      sym(1) = 'Ca'
      sym(2) = 'Ca'
      sym(3) = 'P'
      sym(4) = 'O'
       sym(5) = 'O'
       sym(6) = 'O'
       sym(7) = 'F'
      sym(8) = 'Os'
       sym(9) = 'Os'
       sym(10) = 'Os'
       sym(11) = 'Fs'
DO ix =1 , ncellx*ncelly*ncellz
!     Write all the Ca(1) atoms
            DO index = 1, 4
              iatom = iatom + 1
              write(2,'(a8,i10)') sym(id(index)), iatom
              write(2,'(3g20.10)') &
               xstart + real(ix)*alatt + xfr(index)*alatt, &
               ystart + real(iy)*alatt + yfr(index)*alatt, &
               zstart + real(iz)*clatt + zfr(index)*clatt
            ENDDO
!     Write all the Ca(2) atoms
            DO index = 5,10
              iatom = iatom + 1
              write(2,'(a8,i10)') sym(id(index)), iatom
              write(2,'(3g20.10)') &
               xstart + real(ix)*alatt + xfr(index)*alatt, &
               ystart + real(iy)*alatt + yfr(index)*alatt, &
               zstart + real(iz)*clatt + zfr(index)*clatt
            ENDDO
!     Write all the P atoms
            DO index = 11, 16
              iatom = iatom + 1
              write(2,'(a8,i10)') sym(id(index)), iatom
              write(2,'(3g20.10)') &
               xstart + real(ix)*alatt + xfr(index)*alatt, &
               ystart + real(iy)*alatt + yfr(index)*alatt, &
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            zstart + real(iz)*clatt + zfr(index)*clatt
      ENDDO
!     Write all the O(1) atoms
      DO index = 17 , 22
            iatom = iatom + 1
            write(2,'(a8,i10)') sym(id(index)), iatom
            write(2,'(3g20.10)') &
             xstart + real(ix)*alatt + xfr(index)*alatt, &
             ystart + real(iy)*alatt + yfr(index)*alatt, &
             zstart + real(iz)*clatt + zfr(index)*clatt
      ENDDO
!     Write all the O(2) atoms
      DO index = 23 , 28
            iatom = iatom + 1
            write(2,'(a8,i10)') sym(id(index)), iatom
            write(2,'(3g20.10)') &
             xstart + real(ix)*alatt + xfr(index)*alatt, &
             ystart + real(iy)*alatt + yfr(index)*alatt, &
             zstart + real(iz)*clatt + zfr(index)*clatt
      ENDDO
!     Write all the O(3) atoms
      DO index = 29 , 40
            iatom = iatom + 1
            write(2,'(a8,i10)') sym(id(index)), iatom
            write(2,'(3g20.10)') &
             xstart + real(ix)*alatt + xfr(index)*alatt, &
             ystart + real(iy)*alatt + yfr(index)*alatt, &
             zstart + real(iz)*clatt + zfr(index)*clatt
      ENDDO
!     Write all the F atoms
          DO index = 41, 42
            iatom = iatom + 1
            write(2,'(a8,i10)') sym(id(index)), iatom
            write(2,'(3g20.10)') &
             xstart + real(ix)*alatt + xfr(index)*alatt, &
             ystart + real(iy)*alatt + yfr(index)*alatt, &
             zstart + real(iz)*clatt + zfr(index)*clatt
          ENDDO
!     Write all the Os atoms
          DO index = 43,48
            iatom = iatom + 1
            write(2,'(a8,i10)') sym(id(index)), iatom
            write(2,'(3g20.10)') &
             xstart + real(ix)*alatt + xfr(index)*alatt, &
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                ystart + real(iy)*alatt + yfr(index)*alatt, &
                zstart + real(iz)*clatt + zfr(index)*clatt
              ENDDO
!     Write all the Os atoms
              DO index = 49,54
                iatom = iatom + 1
                write(2,'(a8,i10)') sym(id(index)), iatom
                write(2,'(3g20.10)') &
                 xstart + real(ix)*alatt + xfr(index)*alatt, &
                 ystart + real(iy)*alatt + yfr(index)*alatt, &
                 zstart + real(iz)*clatt + zfr(index)*clatt
              ENDDO
!     Write all the Os atoms
              DO index = 55, 66
                iatom = iatom + 1
                write(2,'(a8,i10)') sym(id(index)), iatom
                write(2,'(3g20.10)') &
                 xstart + real(ix)*alatt + xfr(index)*alatt, &
                 ystart + real(iy)*alatt + yfr(index)*alatt, &
                 zstart + real(iz)*clatt + zfr(index)*clatt
              ENDDO
!     Write all the Fs atoms
              DO index = 67, 68
                iatom = iatom + 1
                write(2,'(a8,i10)') sym(id(index)), iatom
                write(2,'(3g20.10)') &
                 xstart + real(ix)*alatt + xfr(index)*alatt, &
                 ystart + real(iy)*alatt + yfr(index)*alatt, &
                 zstart + real(iz)*clatt + zfr(index)*clatt
              ENDDO
            ENDDO
!     ------------------------------------------------------------
      CLOSE(2)
      ENDPROGRAM cellgen
```

O input CONTROL:

```
#restart
#restart noscale
restart scale
#integrator leapfrog
```

```
#Interatomic Potential Cut offs and specific Ewald algorithm to use
cutoff           8.0000
rvdw cutoff      8.0000
ewald precision  1.0D-6

#Temperature and Pressure, timestep, variable timestep

temperature       300.00
pressure          0.001
#timestep         0.001
variable timestep  0.001
mindis            0.03
maxdis            0.10
#defects    1   1000   1.0
scale  300.00   1000


#Ensemble
#ensemble nve
#ensemble  nvt flang 0.0  0.80  1.86
#ensemble npt hoover 0.1  1.0
#ensemble nvt ber     0.1
ensemble npt ber     1.0  1.0
#pseudo       3.0
#densvar 20


#Number of steps in this run, equil, scale, print, statis, history, rdf
steps             1000
#equilibration         0
print             100
stats             100
#scale               1
#traj      500   500   1
rdf               1000
print rdf
```

job time 172000.00
close time 500.00
finish

O input FIELD:

Potenciais para F-apatita (Mkhonto & de Leeuw, 2002 - J Mater Chem)

units eV

Apatite

nummols 125

atoms 68

Ca 40.078 +2.000 10
P 30.974 +1.180 6
O 15.999 +0.587 24
F 18.998 +1.380 2
Os 0.0000 -1.632 24
Fs 0.0000 -2.380 2

shell 26

17 43 507.40
18 44 507.40
19 45 507.40
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# Dummy P-Os Buckingham potential

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buck 15 45 1200 0.3 0.0
buck 15 46 1200 0.3 0.0
buck 15 48 1200 0.3 0.0
buck 15 49 1200 0.3 0.0
buck 15 50 1200 0.3 0.0
buck 15 51 1200 0.3 0.0
buck 15 52 1200 0.3 0.0
buck 15 54 1200 0.3 0.0
buck 15 55 1200 0.3 0.0
buck 15 56 1200 0.3 0.0
buck 15 57 1200 0.3 0.0
buck 15 58 1200 0.3 0.0
buck 15 60 1200 0.3 0.0
buck 15 61 1200 0.3 0.0
buck 15 62 1200 0.3 0.0
buck 15 63 1200 0.3 0.0
buck 15 64 1200 0.3 0.0
buck 15 66 1200 0.3 0.0
buck 16 43 1200 0.3 0.0
buck 16 44 1200 0.3 0.0
buck 16 45 1200 0.3 0.0
buck 16 46 1200 0.3 0.0
buck 16 47 1200 0.3 0.0
buck 16 49 1200 0.3 0.0
buck 16 50 1200 0.3 0.0
buck 16 51 1200 0.3 0.0
buck 16 52 1200 0.3 0.0
buck 16 53 1200 0.3 0.0
buck 16 55 1200 0.3 0.0
buck 16 56 1200 0.3 0.0
buck 16 57 1200 0.3 0.0
buck 16 58 1200 0.3 0.0
buck 16 59 1200 0.3 0.0
buck 16 61 1200 0.3 0.0
buck 16 62 1200 0.3 0.0

buck 16 63 1200 0.3 0.0
buck 16 64 1200 0.3 0.0
buck 16 65 1200 0.3 0.0

buck 11 68 1200 0.3 0.0
buck 11 67 1200 0.3 0.0
buck 12 68 1200 0.3 0.0
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buck 13 68 1200 0.3 0.0
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buck 14 67 1200 0.3 0.0
buck 15 68 1200 0.3 0.0
buck 15 67 1200 0.3 0.0
buck 16 68 1200 0.3 0.0
buck 16 67 1200 0.3 0.0

angles 36

harm 17 11 23 1.322626 109.47
harm 17 11 29 1.322626 109.47
harm 17 11 35 1.322626 109.47
harm 23 11 29 1.322626 109.47
harm 23 11 35 1.322626 109.47
harm 29 11 35 1.322626 109.47
harm 18 12 24 1.322626 109.47
harm 18 12 30 1.322626 109.47
harm 18 12 36 1.322626 109.47
harm 24 12 30 1.322626 109.47
harm 24 12 36 1.322626 109.47
harm 30 12 36 1.322626 109.47
harm 19 13 25 1.322626 109.47
harm 19 13 31 1.322626 109.47
harm 19 13 37 1.322626 109.47
harm 25 13 31 1.322626 109.47
harm 25 13 37 1.322626 109.47
harm 31 13 37 1.322626 109.47
harm 20 14 26 1.322626 109.47
harm 20 14 32 1.322626 109.47
harm 20 14 38 1.322626 109.47
harm 26 14 32 1.322626 109.47
harm 26 14 38 1.322626 109.47
harm 32 14 38 1.322626 109.47
harm 21 15 27 1.322626 109.47
harm 21 15 33 1.322626 109.47

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harm 21 15 39 1.322626 109.47
harm 27 15 33 1.322626 109.47
harm 27 15 39 1.322626 109.47
harm 33 15 39 1.322626 109.47
harm 22 16 28 1.322626 109.47
harm 22 16 34 1.322626 109.47
harm 22 16 40 1.322626 109.47
harm 28 16 34 1.322626 109.47
harm 28 16 40 1.322626 109.47
harm 34 16 40 1.322626 109.47

finish
close
```

Outras informações:

Durante o desenvolvimento do projeto meu desempenho acadêmico se manteve constante, uma das dificuldades encontradas no projetos foram, entre outras, uma explicação escassa dos métodos utilizados para computar o valor dos potenciais que entrariam no arquivo FIELD, foi usado como base o artigo (7), mas o mesmo não explicava de maneira eficiente como entrar com esses potenciais no arquivo FIELD. Esse foi um dos motivos que atrasou as metas do projeto. Além disso após o entendido como gerar o arquivo FIELD, por ser uma molécula com muitos graus de liberdade está sendo difícil estabilizar a mesma, pois isso depende dos potenciais entre os átomos e os mesmos são numerosos.

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Não consegui falar com o oriendator essa semana para colocar a opinião do mesmo.