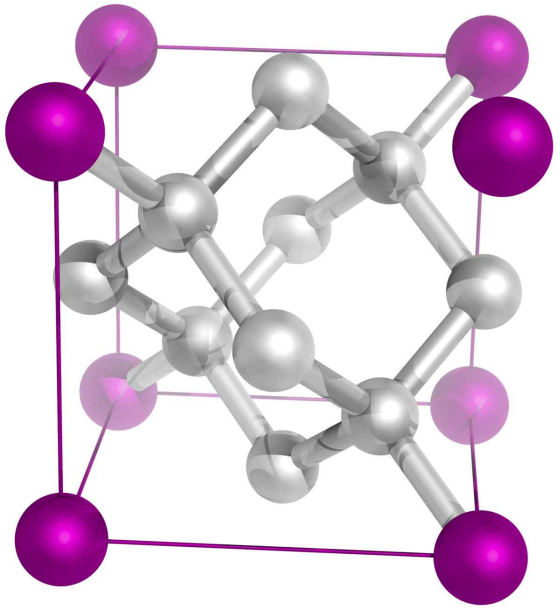
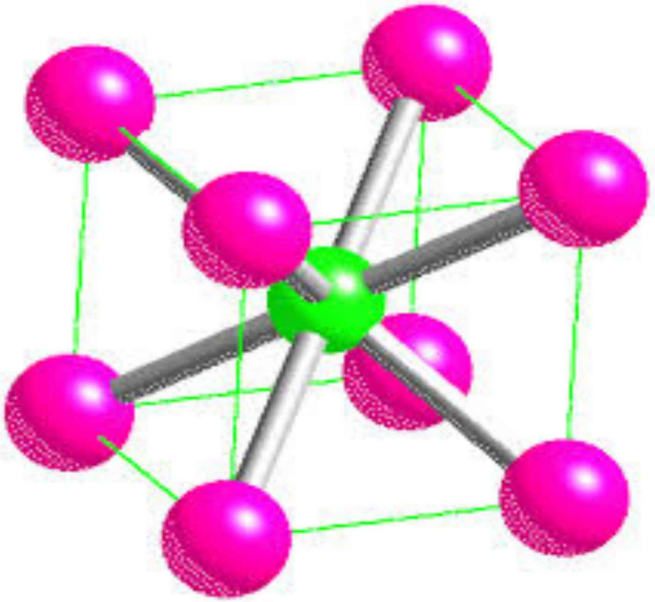
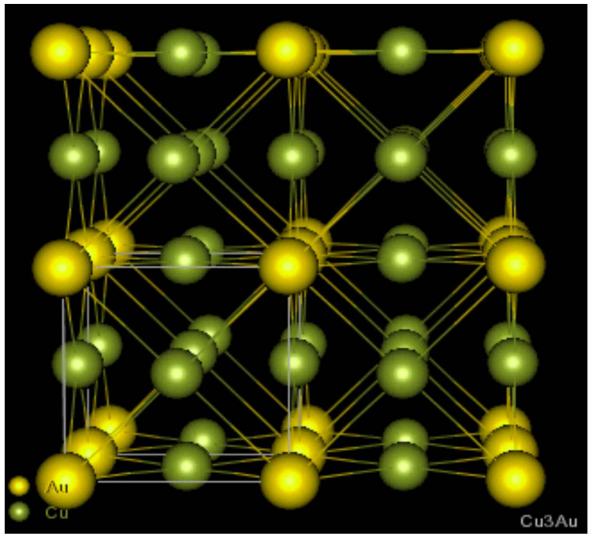
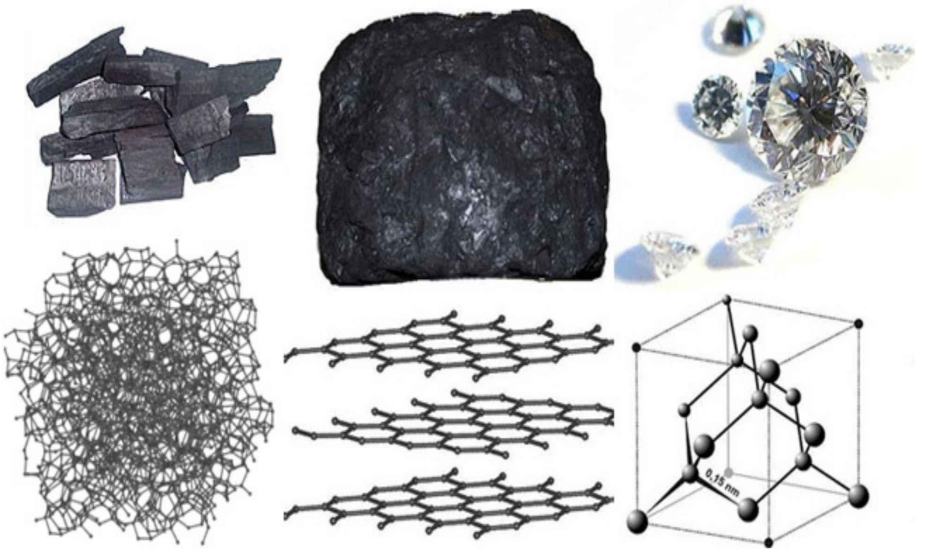
Sistemas Cristalinos: Redes Periódicas



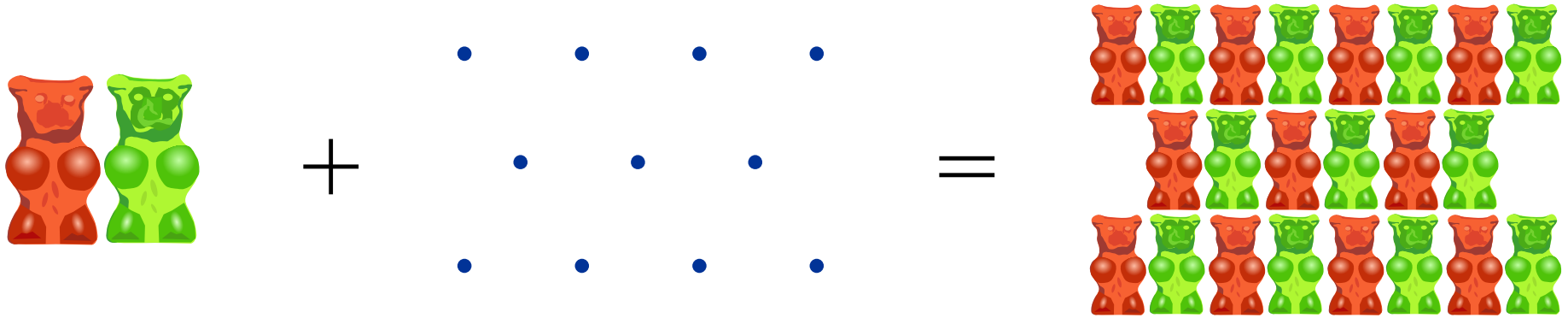






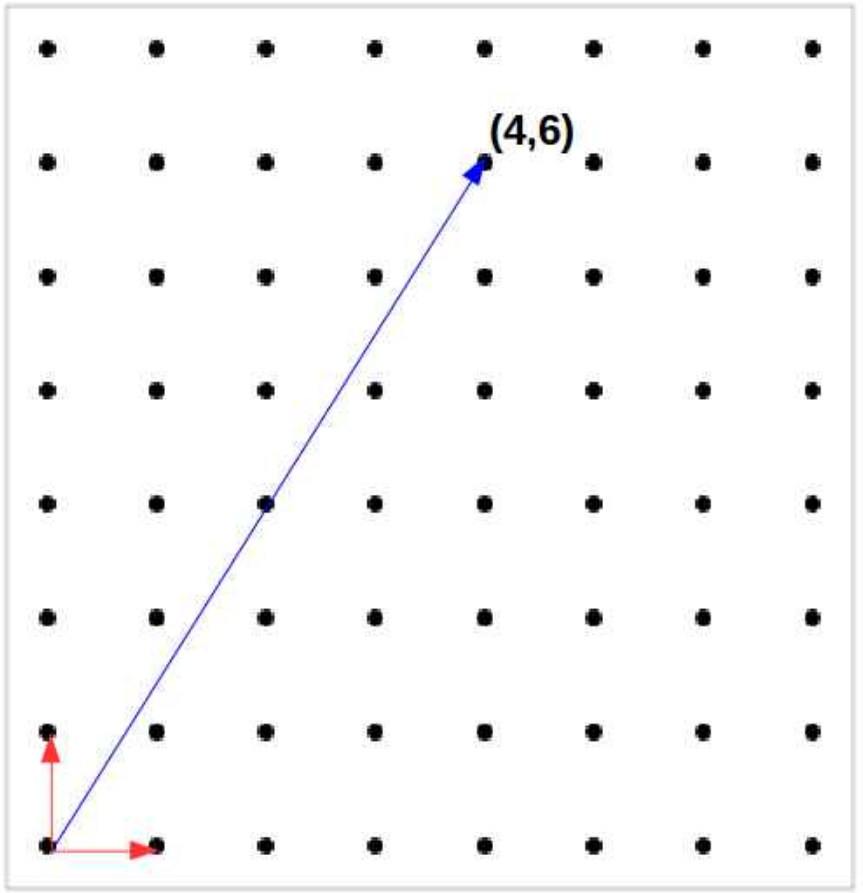
Sistemas Cristalinos: Redes Periódicas

"Um cristal do ponto de vista geométrico é definido como a junção de uma base e uma rede periódica"

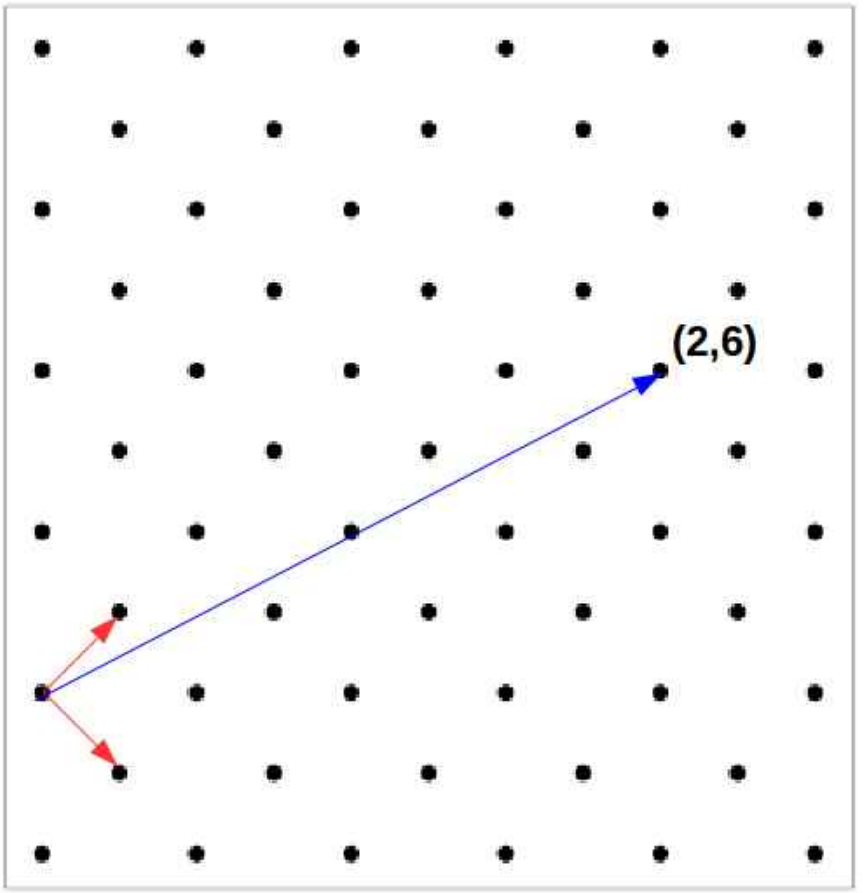


basis lattice crystal

Redes Periódicas: Rede Quadrada



uprigth square lattice



diagonal square lattice

Vetores de rede: a1 e a2

a1 = (1,0)
a2 = (0,1)

R=4a1+6a2

Vetores de rede: a1 e a2

a1 = (√2/2,-√2/2)
a2 = (√2/2,√2/2)

R=2a1+6a2

Programa Básico em Fortran90

rede_quadrada.f90

```
PROGRAM squarelattice
IMPLICIT NONE
! Esse programa cria uma rede bidimensional periodica.

REAL*8 :: latt1(3),latt2(3)
INTEGER, PARAMETER :: maxim=50
REAL*8 :: x, y, z
INTEGER :: i1,i2

OPEN(UNIT=10, FILE='saida0.dat', STATUS="NEW")
OPEN(UNIT=11, FILE='saida1.dat', STATUS="NEW")
OPEN(UNIT=12, FILE='saida2.dat', STATUS="NEW")
```

Cabeçalho do programa: Declaração de Variáveis, Funções, arquivos, etc..

Programa Básico em Fortran90

Definições.... (vetores de rede)

```
DATA latt1/1.0d0, 0.0d0, 0.0d0/
DATA latt2/0.0d0, 1.0d0, 0.0d0/
```

Loops.... (repetições)

```
DO i1=0, maxim
DO i2=0, maxim

x=i1*latt1(1)+i2*latt2(1)
y=i1*latt1(2)+i2*latt2(2)
z=i1*latt1(3)+i2*latt2(3)

!Exemplo de formatacao livre
WRITE(10,*) 'C',x, y, z
!Exemplo de formatacao usando o descritor F
WRITE(11,"(A,3F16.4)") 'C',x, y, z
!Exemplo de formatacao usando o descritor E
WRITE(12,"(A,3E16.4)") 'C',x, y, z


END DO
END DO
```

Programa Básico em Fortran90

Fim....

```
END DO
END DO

CLOSE (UNIT=10)
CLOSE (UNIT=11)
CLOSE (UNIT=12)

END PROGRAM squarelattice
```

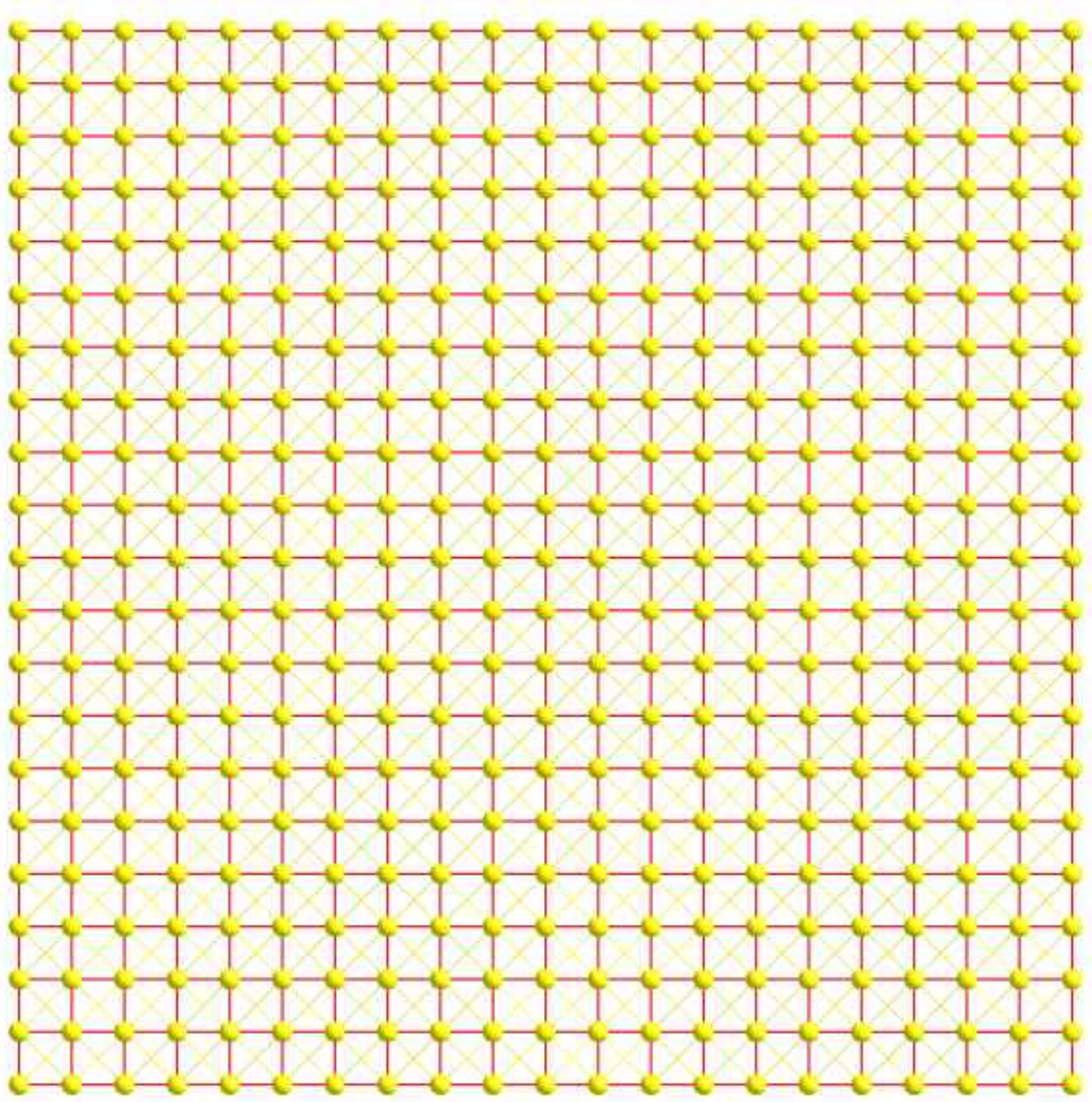
Programa Básico em Fortran90

*rede_quadrada.f90

```
PROGRAM squarelattice
IMPLICIT NONE
! Esse programa cria uma rede bidimensional periodica.
REAL*8 :: latt1(3),latt2(3)
INTEGER, PARAMETER :: maxim=50
REAL*8 :: x, y, z
INTEGER :: i1,i2

OPEN(UNIT=10, FILE='saida0.dat', STATUS="NEW")
OPEN(UNIT=11, FILE='saida1.dat', STATUS="NEW")
OPEN(UNIT=12, FILE='saida2.dat', STATUS="NEW")

DATA latt1/1.0d0, 0.0d0, 0.0d0/
DATA latt2/0.0d0, 1.0d0, 0.0d0/

DO i1=0, maxim
DO i2=0, maxim

x=i1*latt1(1)+i2*latt2(1)
y=i1*latt1(2)+i2*latt2(2)
z=i1*latt1(3)+i2*latt2(3)

!Exemplo de formatacao livre
WRITE(10,*) 'C',x, y, z
!Exemplo de formatacao usando o descritor F
WRITE(11,"(A,3F16.4)") 'C',x, y, z
!Exemplo de formatacao usando o descritor E
WRITE(12,"(A,3E16.4)") 'C',x, y, z

END DO
END DO
CLOSE (UNIT=10)
CLOSE (UNIT=11)
CLOSE (UNIT=12)
END PROGRAM squarelattice
```

35 linhas de código...

Rede periódica gerada...



maxim=20