VIIth International Conference
Channeling 2016
Sept. 24-30. Sermione, Desenzano del Garda, Italy

Correlations in thermal vibrations of crystal atoms. Effect on dechanneling and bremsstrahlung

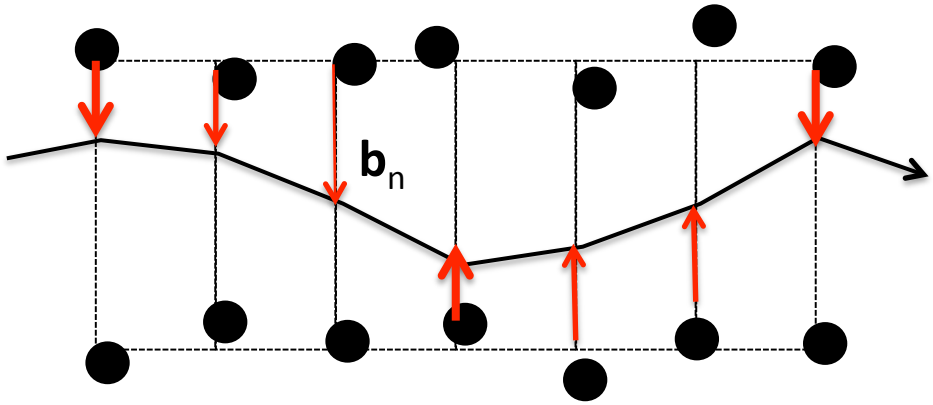
Xavier Artru
Institut de Physique Nucléaire de Lyon (France)

Effect of crystal vibrations in channeling

We know that in a crystal the atoms vibrate about their mean positions $\langle \mathbf{R}_n \rangle$ ($\mathbf{n} = \{n_1,n_2,n_3\}$ = lattice site). The *displacements* are $\mathbf{u}_n(t) = \mathbf{R}_n(t) - \langle \mathbf{r}_n \rangle$.
The vibrations reduce X-ray and neutron diffraction by the Debye-Waller factor

$$\exp(-\langle \mathbf{u}^2 \rangle \mathbf{q}^2),$$ where $\mathbf{q}$ = momentum transfer in units hbar = 1.

In channeling, the vibrations reduce the depth of the potential well and increase the number of incoherent scatterings which cause dechanneling, re-channeling and volume capture.
These processes can be simulated on computers using the *binary collision* method which builds the particle trajectory cell by cell :



In each cell, the particle pomentum is changed by $\mathbf{q}(\mathbf{b}_n)$ where $\mathbf{b}_n = \mathbf{r} - \mathbf{u}_n(t)$.

$\mathbf{u}_n(t)$ is generated at random.
According to which law ?

How do atomic chains vibrate ?

The atom displacements $\mathbf{u_n}(t)$ can be decomposed in phonons:

$$\mathbf{u_n}(t) = \sum_{\mathbf{k}} \sum_{\hat{\mathbf{e}}} \mathrm{Re}\{\, a(\mathbf{k},\hat{\mathbf{e}})\, \hat{\mathbf{e}}\, \exp[\, i\mathbf{k}.\mathbf{R}_n - i\omega(\mathbf{k},\hat{\mathbf{e}})t\,]\, \}$$

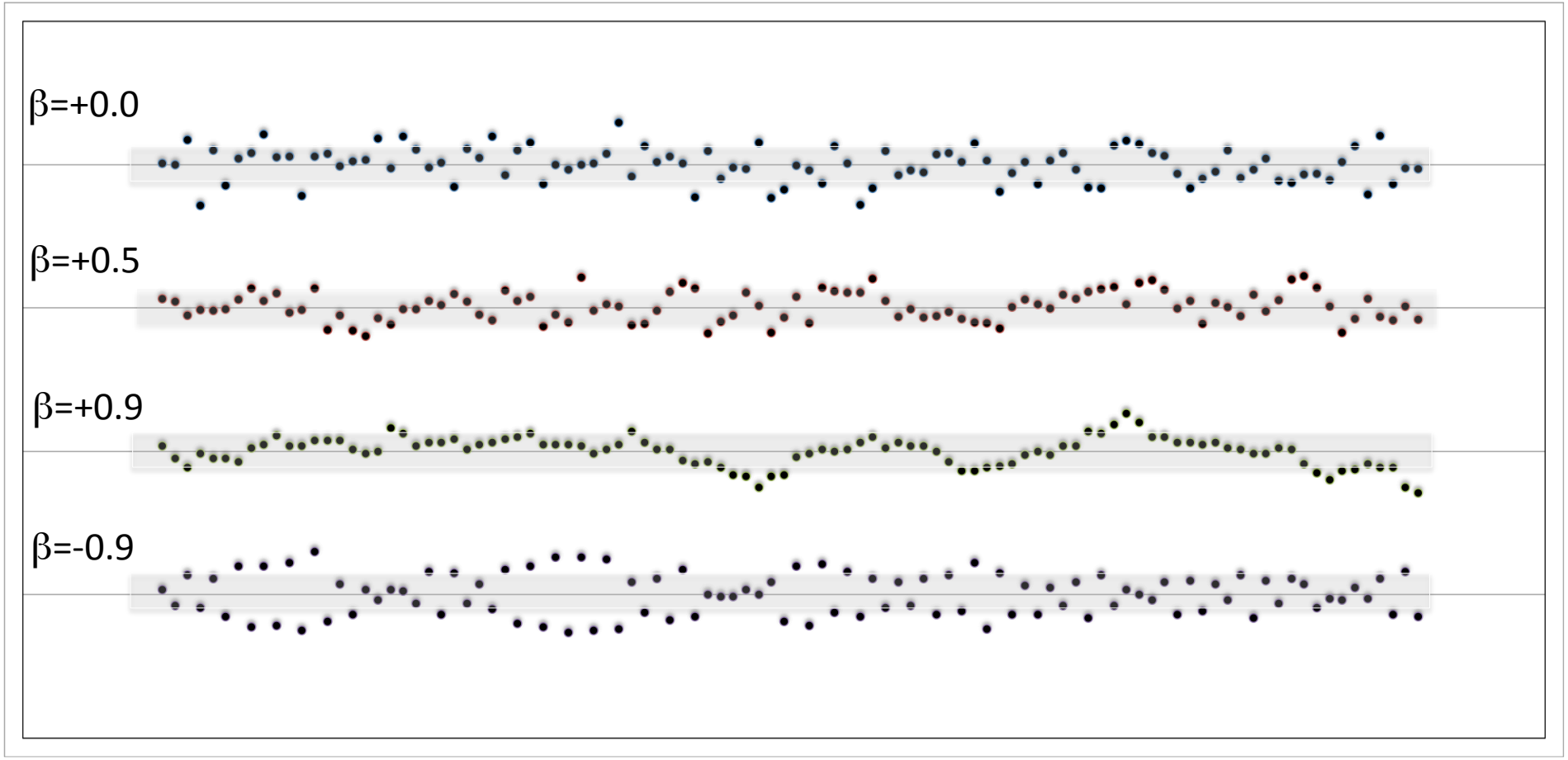
In usual channeling simulations, the amplitude of this vibration is characterized only by the r.m.s. displacement $\langle \mathbf{u}^2 \rangle$.
$\langle \mathbf{u}^2 \rangle$ increases with temperature, while being nonzero at T=0 (‘‘zero point motion’’).

Phonons of long wavelengths incite the neighbouring atoms to vibrate in the same direction. Thus the vibrations of neighbouring atoms are correlated : $\langle \mathbf{u_m} \cdot \mathbf{u_n} \rangle \neq 0$.
In a simple model, presented later :

$$\langle \mathbf{u_m} \cdot \mathbf{u_n} \rangle = \beta^{|m-n|} \langle \mathbf{u}^2 \rangle \qquad |\beta| < 1$$

The parameter β characterizes the both the *strenght* and the *range* of the correlation.

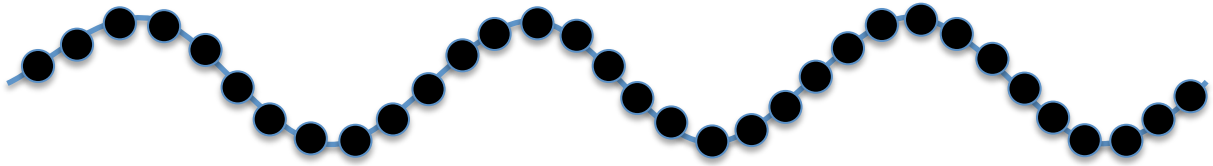
Atomic chain vibration (simulated)



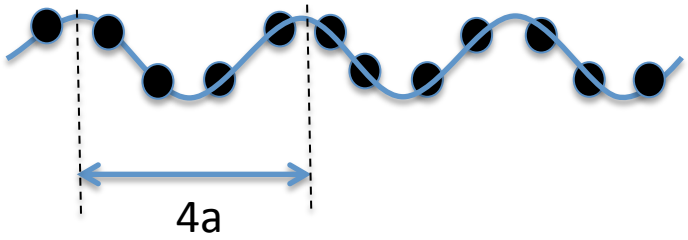
Decomposition of $\mathbf{u}_n(t)$ in phonons :

a = atomic spacing
$k = 2\pi/\lambda$

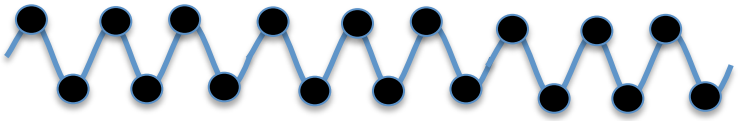
long wavelength
$\lambda \sim 10\ a$



medium wavelength : $\lambda \sim 4a$
-> $\beta \sim \exp(-1) \sim 0.4$



min. wavelength : $\lambda = 2a$

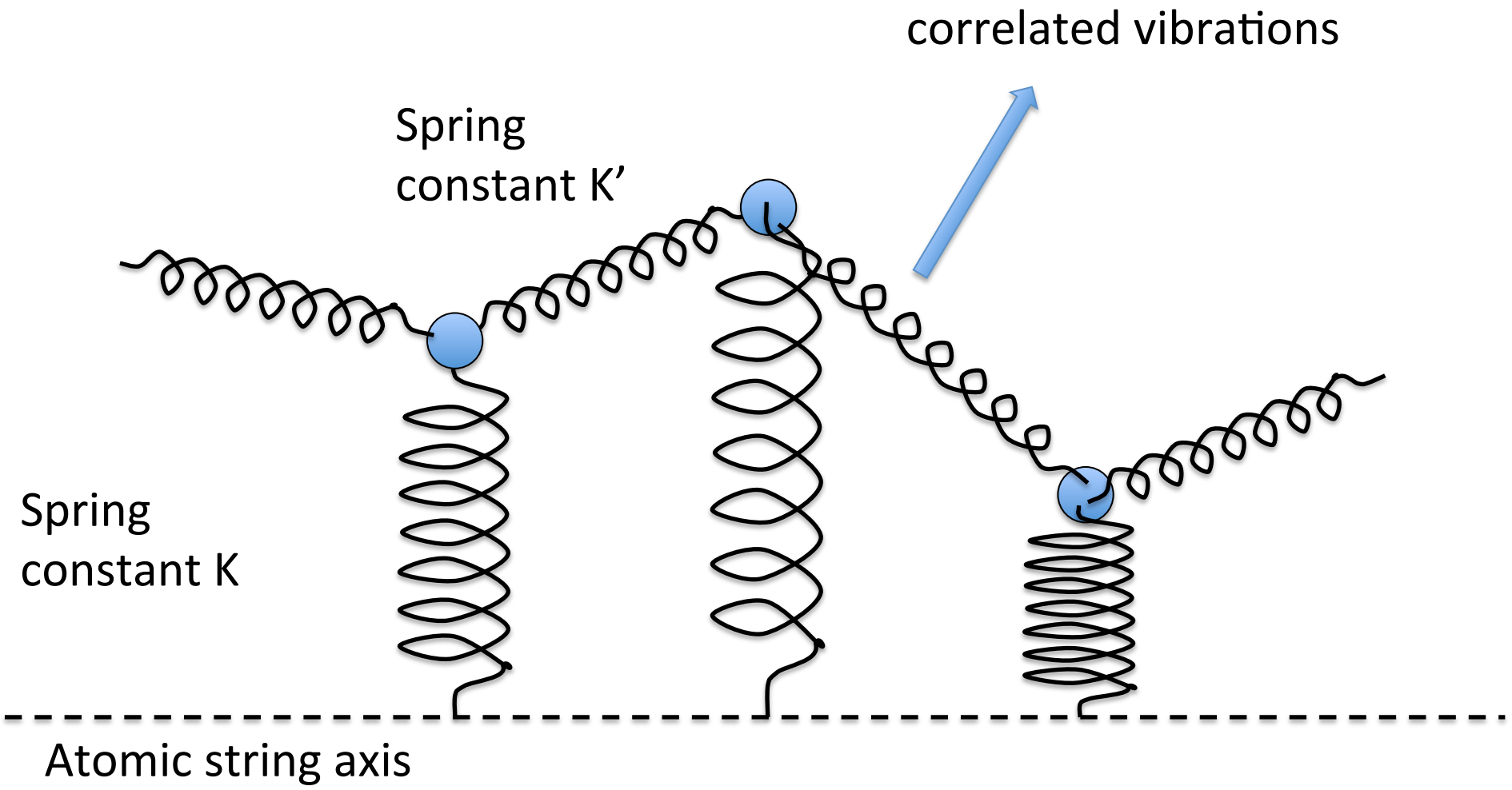


Bose-Einstein statistics :

$$\langle \mathbf{u}^2 \rangle \approx (\rho_A\, m_A)^{-1} \int d^3\mathbf{k}/\omega \quad \{ 1/2 + 1/[\exp(\omega/kT)-1] \}$$

For long wavelength, the integrand is $\sim$ Cte $\times$ $d|\mathbf{k}| \times d\Omega_{\mathbf{k}}$

S*p*ring model for the atomic s*t*ring vibration



Monte Carlo simulation

Random drawing of the transverse positions $\mathbf{u}_1$, $\mathbf{u}_2$, **….** , $\mathbf{u}_n$, ... of the atoms :

- ***Without*** correlations : draw each $\mathbf{u}_n$ independently, with the Gaussian distribution

$$P(\mathbf{u}_n) = (2\pi\langle \mathbf{u}^2\rangle)^{-1} \exp\{ - \mathbf{u}_n^2 / \langle \mathbf{u}^2\rangle \} \qquad (1) \qquad \mathbf{u} = (x,y)$$

- ***With*** correlations : - draw $\mathbf{u}_1$ with (1)

  - draw $\mathbf{u}_2$, $\mathbf{u}_3$, **….** recursively with the distribution

$$P(\mathbf{u}_{n+1}) = C/(2\pi) \exp\{ - C (\mathbf{u}_{n+1} - \beta \mathbf{u}_n)^2 \}$$

β measures the strength of the correlation. $|\beta| < 1$.
C is given by $C^{-1} = (1 - \beta^2) \langle \mathbf{u}^2\rangle$.

Thus, $\langle \mathbf{u}_{n+1}\rangle = \beta \mathbf{u}_n$ for given $\mathbf{u}_n$ and $\langle \mathbf{u}_m \cdot \mathbf{u}_n\rangle = \beta^{|m-n|} \langle \mathbf{u}^2\rangle$,

The *correlation length* is $\lambda_C = a/\mathrm{Log}(\beta^{-1})$; $\lambda_C \to \infty$ for $\beta \to 1$.

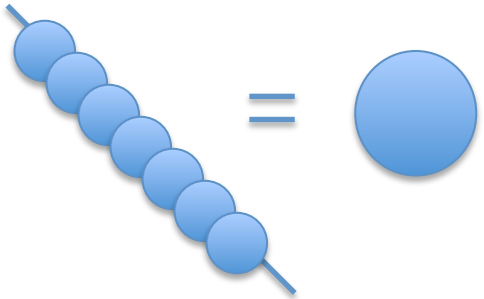
Effect of the correlations on dechanneling

A group of N successive and nearly aligned atomic nuclei scatters an **aligned** particle beam *as strongly as one* ***super-nucleus*** *of charge N×Z* .

The mean square momentum transfer is

$$\langle \mathbf{q}^2 \rangle = N^2 \langle \mathbf{q}_1^2 \rangle ,$$

intead of $N \langle \mathbf{q}_1^2 \rangle$ for non-aligned nuclei.



Classical explanation : $\mathbf{q} = \sum_n \mathbf{q}_n$; $\mathbf{q}_n \approx 2\, Z\alpha\ \mathbf{b}_n / b_n^2$;

$\mathbf{b}_n$ = impact parameter = $\mathbf{r}_{particle} - \mathbf{u}_n$ (α =1/137)

The alignment requirement is $|\mathbf{u}_n - \mathbf{u}_m| \ll |\mathbf{b}|$

In reality, N is limited by non-perfect alignment of the beam and the trajectory bending.

Dechanneling simulation (for axially channeled e^-)

Momentum transfer from 1 atom : atomic screening

$$\mathbf{q}(\mathbf{b}) = - 2Z\alpha \left[(b^2 + r^2_{nucleus})^{-1} - (b_n^2 + r^2_{atom})^{-1} \right] \mathbf{b}$$

Channeling potential :

Ideal atomic string : $U(\mathbf{b}) = (Z\alpha/a) \; \mathrm{Log} \{ (b^2 + r^2_{nucl.}) / (b_n^2 + r^2_{atom})) \} + \mathrm{Cte}$

After convolution with atom vibrations :

$$U(\mathbf{b}) \approx - (Z\alpha/a) \; \mathrm{Log} \{ (b^2 + r^2_{nucl.} + \langle \mathbf{u}^2 \rangle_{th}) / (b_n^2 + r^2_{atom} + \langle \mathbf{u}^2 \rangle_{th})) \}$$

(form used by Baier, Katkov and Strakhovenko)

Simulation of the electron motion by ***binary collision*** :

$$\mathbf{v}_{n+1} = v_n + E^{-1} \mathbf{q}(\mathbf{b}_n) \quad \text{with} \quad \mathbf{b}_n = \mathbf{r}_n - \mathbf{u}_n$$

$$\mathbf{r}_{n+1} = \mathbf{r}_n + a \, \mathbf{v}_n$$

Numerical results

Parameters :

Z = 14 (Si)
$r_{nucl.}$ = 1 fm
r_{atom} = 0.05 nm
a = 0.2 nm
$\langle \mathbf{u}^2 \rangle = (0.0042\ \text{nm})^2$
E = 100 MeV

- Incidence angle : $\mathbf{v}_{in} = 0$
- Incidence points : $|\mathbf{r}_{in}| = (a/20) \times k$ (k = 0, 1, … 9)
  (transverse energies between - 481 eV and - 4 eV)

We define the ***dechanneling length*** $L_d = n_d \times a$ in two ways :

> n_{d1} = No of the **first** binary collision after which $E_T > U(a/2)$

> n_{d2} = No of the first binary collision after which $r_n > a/2$ (= 0.1nm)

Results :

β	$\langle n_{d1} \rangle$	$\langle n_{d2} \rangle$	reduction
0.	546	1629	
0.5	491	1470	10 %
0.9	391	1174	28 %
- 0.9	516	1564	4 or 5 %

Results at nonzero incidence angle

Incidence angle : $\mathbf{v}_{in} = 10^{-3}$ ($\approx 1/3\ \theta_{Lindhard}$)
Incidence points : $|\mathbf{r}_{in}| = (a/20) \times k$ (k = 0, 1, … 4)
(transverse energies between - 431 eV and - 22 eV)

Results :

β	$<n_{d1}>$	$<n_{d2}>$	reduction
0.	678	1784	
0.5	600	1617	~ 10 %
0.9	464	1297	~ 30 %
- 0.9	630	1681	6 or 7 %

Quantum approach

Consider N successive atomic nuclei of transverse positions $\mathbf{u}_n$, $\mathbf{u}_{n+1}$, …. , $\mathbf{u}_{n+N}$

In the Born approximation, the scattering cross section by this group is

$$(d\sigma /d^2\mathbf{q})_{group} = (d\sigma/d^2\mathbf{q})_{1\text{-atom}} \times |F(\mathbf{q})|^2$$

with $F(\mathbf{q}) = \Sigma_1^N \exp(i\, \mathbf{q}.\mathbf{r}_n)$

$$|F(\mathbf{q})|^2 = N + \Sigma_{n \neq m} \exp[i\, \mathbf{q}.(\mathbf{r}_n - \mathbf{r}_m)]$$

interferences

When $|\mathbf{r}_n - \mathbf{r}_m| < 1/q$ the interference term is **positive.**
In our Monte-Carlo model,

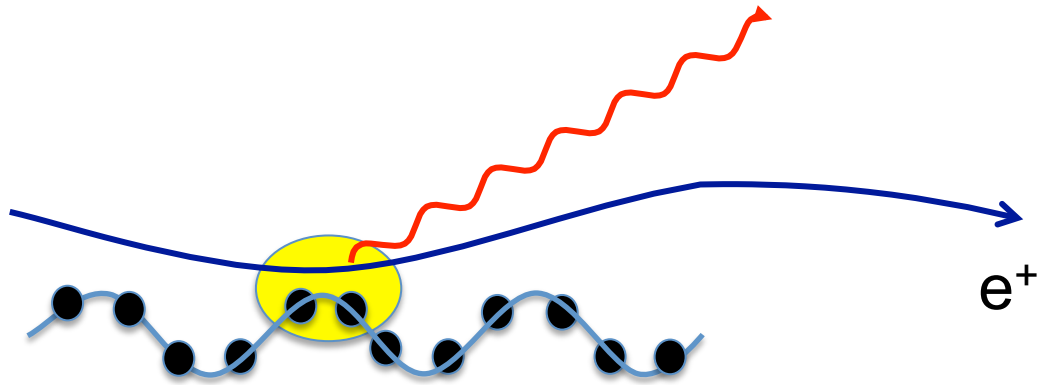
$$<|\mathbf{r}_n - \mathbf{r}_m|^2> = 2 <\mathbf{u}^2> \times (1-\beta^{|n-m|})$$

$$\rightarrow \quad |F(\mathbf{q})|^2 = \Sigma_{n,m} \exp\{ - (1-\beta^{|n-m|}) <\mathbf{u}^2> \mathbf{q}^2 \}$$

The larger is β, the stronger is scattering.

Semi-coherent bremsstrahlung

Since the scattering is stronger, the **Bremsstrahlung** is also be more powerfull (compared with simulation without correlation).



Atoms **m** and **n** interfere if their distance $d = a \times |m-n|$ is less than

- the *coherence* length $l_C \sim \gamma^2 / \omega_{photon}$.
- the *correlation* length λ_C of atom vibrations

The result is a "*Semi-coherent bremsstrahlung*" (SCB)

This "semi-coherence" is not taken into account in ordinary Coherent Bremsstrahlung:

- CB is submitted only to the first condition,
- CB is attenuated by the Debye-Waller factor, while SCB is attenuated by $|F(\mathbf{q})|^2$, which has a slower decrease.

Conclusions

- The correlations between the vibrations of neighbouring atoms decrease the dechanneling length (for a given value of $<\mathbf{u}^2>$).

  This is shown both in classical approach (binary collision model) and in the quantum Born approximation.
- An effect of ~ 30% could occur if the phonon spectrum contains a significant part of long waves.
- Since the scattering is stronger, the Bremsstrahlung should be more powerfull (compared with simulation without correlation). We have a '*semi-coherent*' bremsstrahlung.
- Precise simulations with a more realistic model of atom vibrations are needed.

Thank you !