Can nano-particles of Ice and Dust affect the Charge-Exchange X-ray emission?

V. Kharchenko

Harvard-Smithsonian CfA & University of Connecticut

1. Nano-particles in Astrophysical Environments
2. Interaction between nano-particles and astrophysical plasmas
3. Nucleation of nano-scale dust, ice, and haze particles around ion seeds. Size distribution of nano-particles
4. Charge exchange, scattering, and fluorescence phenomena for nano-scale objects
5. Multi-channel collisions between ions and nano-particles and charge-exchange. Fragmentation of nano-particles
6. Theory and experiments on charge-exchange processes in collisions between highly charged ions and nano-particles
Circumstellar Dust in Accretion Disks
Example: Accretion disk of the red dwarf AU Mic. Webb observations. Very strong stellar wind.

Zodiacal Dust

Nano-particles: Interstellar dust, Cometary ice and dust, Noctilucent clouds, Exoplanetary dust and haze, aerosols etc.
Cometary Dust and Ice Particles, Exoplanetary Atmospheric Haze, Aerosols, and High Altitude Clouds

Cometary Dust

Interstellar Dust

Weingartner & Draine (2001) model for Milky Way dust

$R_V = 3.1$

PAH C/H=56 ppm

Particle size [μm]

$\nu = 6 \times 10^{-7}$ cm$^3$/H

silicate

carbon/PAH

carbonaceous material

iron sulfide

silicate glass

Credit: Megumi Matsumoto et al

200 nm
Charge Transfer Collisions between Nanoparticles and Ions: Hybrid Model

(This equation is valid for the single electron capture in quasi-elastic collisions between ion and nanoparticle)

\[
\sigma_{CX}(a, E, I_p) = \frac{\pi}{2} \left[ a + (1 + 2\sqrt{q}) \frac{e^2}{I_p} + \left( \frac{\hbar^2}{2m_e I_p} \right)^{\frac{1}{2}} \left( \ln \left( \sqrt{\frac{E_0}{E}} \right) + A_q \right) \right]^2,
\]
Contribution of Zodiacal Dust into the local X-ray background

Size Distribution of nano-particle radius $a$:

\[
\frac{\partial n(r, a)}{\partial a} \simeq 2.5 n_d(R_0) \frac{a_{\text{min}}^{3.5}}{a^{3.5}} \left(\frac{R_0}{r}\right)^2
\]

where

- $R_0 = 1\text{AU}$;
- $n_d(R_0) = 1.5 \times 10^{-10} \text{ cm}^{-3}$,
- $I_0(\hbar\omega)$ is the photon flux at $R_0$.

Nano-size dust particles can be trapped in the region $\sim (0.1 - 0.2) R_0$ and CX collisions between ions SW and nano particles may create neutral SW wind of H and He $^+$:

\[
\Gamma(\text{He}^+) = \langle n_d(r,a)\sigma_{\text{CX}}^{\text{He}^+}(a) \rangle_{r,a} = 1.7 \times 10^{-21}\text{ cm}^{-1}
\]

*In situ* satellite observations: $4.6 \times 10^{-21}\text{ cm}^{-1}$

(Collier et al. 2003).

The estimated value of the total X-ray flux from grains is smaller two orders of magnitude than the X-ray background emission. It can be seen during X-ray Solar Flares.

Relative intensity of X-rays $I_Z/I_0$ induced by Zodiacal Dust for photons with different energies:

- $I_z/I_0$ [10$^{-8}$] vs Photon Energy [eV]
- Lewkow 2016 (Springer)

- $I_z/I_0$ vs $r$ (Sun)
Cometary X-rays above 1KeV: Possible Contribution of the Dust/ Gas Scattering

![Graph showing comparison of modeled spectral intensity contributions](image)

**Figure 1.** Comparison of the modeled spectral intensity contributions from CX and dust/ice particle scattering to the *Chandra* observation of Comet Ikeya–Zhang. The modeled scattering emission includes dust contribution from all grain radii. The scattering model is calculated for both the average solar and solar flare spectrum, with the solar flare spectrum producing an excellent agreement to the observation at energies greater than 1 keV.

Fig. 3.11 Comparison of X-ray spectrum from comet Ikeya-Zhang [10] and Jupiter [3], observed during solar X-ray flares. The data sets have been scaled to overlay together in order to better visualize the strong similarity in spectral structure between the two astronomical objects at photon energies above 1 keV.
New Model for CX collisions between Ions and Nano-particles:
Charge Exchange in collisions of $C_{60}$ fullerene with $N^+$ ions (Experiment and Theory)

$C_{60} + N^+ \rightarrow N + C_{60} - 2m + m \ast C_2$

$m$ – the number of ejected $C_2$ molecules

**Figure 6.7:** The experimental cross sections$^{[3]}$ for $C_{60}$ colliding with $N^+$ (shown as the circular, square, triangular and diamond points) plotted along side our model (shown in black).

Charge Exchange collisions between $C_{60}$ fullerene and $O^+$ ion: Experiment and Theory


Figure 6.6: The experimental cross sections\cite{Christian} for $C_{60}$ colliding with $O^+$ (shown as the circular, square, triangular and diamond points) plotted along side our model (shown in black).
Multi-electron Capture in Collisions of Nano-Particles and Highly Charged Ions

\[ C_{60} + Ar^{8+} \rightarrow Ar^{*(8-m)+} + \ldots \]

**Experimental data:**

**Theoretical results:**

Impact Parameter ("Capture Radius")
Stripping of O and S ions in collisions with nano particles

Incoming Ion $X^{q+}$ \rightarrow \text{Nano-size particle} \rightarrow \text{Outgoing ion} $X^{q\pm m}$

Electron capture or Stripping

Thin films experiments

$<q_{final}>$

Beam energy (Mev/u)

Carbon films ~10 - 50nm

"Highly Charged Ion – Induced Water Cluster Fragmentation “

Maisonny et al., ICPEAC 2011, Conference Series 388(2012)

Size “n” of Water Cluster \((\text{H}_2\text{O})_n\text{H}^+\)

- \(\text{Xe}^{20+} (300 \text{ keV})\)
- \(\text{O}^{3+} (37.2 \text{ keV})\)
- \(\text{He}^{2+} (30 \text{ keV})\)
Dynamics of nucleation and particle size distribution: Example of $\text{Ar}_n\text{H}^+$ nucleation

Ice Particle Nucleation and Solvation Shells

Water molecules $\text{H}_2\text{O}$

Ion Mediated Nucleation of Ice and Haze Nano-particles

MD Simulations of cluster growth

COLLISIONAL REACTIONS: Example

$X^q+$ Highly Charge ion

$X^{*(q-1)+}$ Exited “High q” Ion

Various nanoparticle products: $m*C_2$, methane, benzine etc. and their ions
Reactive and Inelastic Collisions between Nano-Particles and Ions

Example:

\[ C_{60} + q^+ \rightarrow C_{60} - 2m + X(q - 1)^+ + m * C_2 \]

Initial State Energies

Final State Energies

INTERPARTICLE DISTANCE [arb. units]

STAT ENERGY [arb. units]

Statistical aspects of ultracold resonant scattering

Michael Mayle, Brandon P. Ruzic, and John L. Bohn
JILA, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado 80309-0440, USA
State’s “RANDOM WALK” during Collisions between Nano-Particles and Ions

Example of Two Trajectories

Region of efficient transitions between Initial and Final States
Time Evolution of State Population: From Random Walk to Diffusion in Energy Space

15 Steps of Random Walk Inside Reaction Region

Diffusion-like Regime

Initial Population

State Number (Index)

L=1 : m= -1, 0, 1
Simulations were performed for simplified $O^{8+} + (H_2O)_n$ model. Number of molecules in the initial water cluster is $n=100$. 
CONCLUSIONS

• Highly charged ions can induce X-rays in collisions with dust or Ice nano-particles.
• Intensity and spectra of emitted X-rays strongly depend on collision velocity as well as on a particle size and material.
• Nano particle can be very efficient in stripping energetic ions and neutral atoms (Jupiter-like mechanism).
• Stellar or Solar Wind ions induces fragmentations of Ice/dust particles and stimulate growth of new small grains.
• Dust and Ice nano-particles can be simultaneously involved in different mechanisms of X-ray production.
Nucleation of $\text{Ar}_n\text{H}^+$ Nano-Clusters in Ar gas
$\text{Ar}_4\text{H}^+ : \text{Single Ar}$

- **Simulation Ensemble Average**
- **Theoretical Average from Eq. 1**

- **Y-axis:** Average Internal KE (eV)
  - Range: 0.06 to 0.001

- **X-axis:** Time since formation (ps)
  - Range: 0 to 800 ps
Kinetic Energy in C60 + C60+ Collisions

**Figure 5.5:** The nuclear kinetic energy as a function of time taken from one of the QMD simulations of the collision between C$_{60}$ and C$_{60}^+$. This simulation had a collision energy of 200 eVs and an impact parameter of 12.28 $a_0$.

**Figure 5.6:** The nuclear kinetic energy as a function of time taken from one of the QMD simulations of the collision between C$_{60}$ and C$_{60}^-$. This simulation had a collision energy of 409 eVs and an impact parameter of 14.17 $a_0$. 


C60 + C60+ Charge Transfer
Figure 1.1: Geometry of C$_{60}$ and the electron probability isosurface calculated using density functional theory (DFT)$^1$
Figure 5.3: The optimized geometry for the C$_{60}$ dimer calculated using density functional theory.
Statistical aspects of ultracold resonant scattering

Michael Mayle, Brandon P. Ruzic, and John L. Bohn
JILA, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado 80309-0440, USA
Figure 6.8: The experimental cross sections\textsuperscript{[2]} for C\textsubscript{60} colliding with Ne\textsuperscript{+} (shown as the circular, square, triangular and diamond points) plotted alongside our model (shown in black).