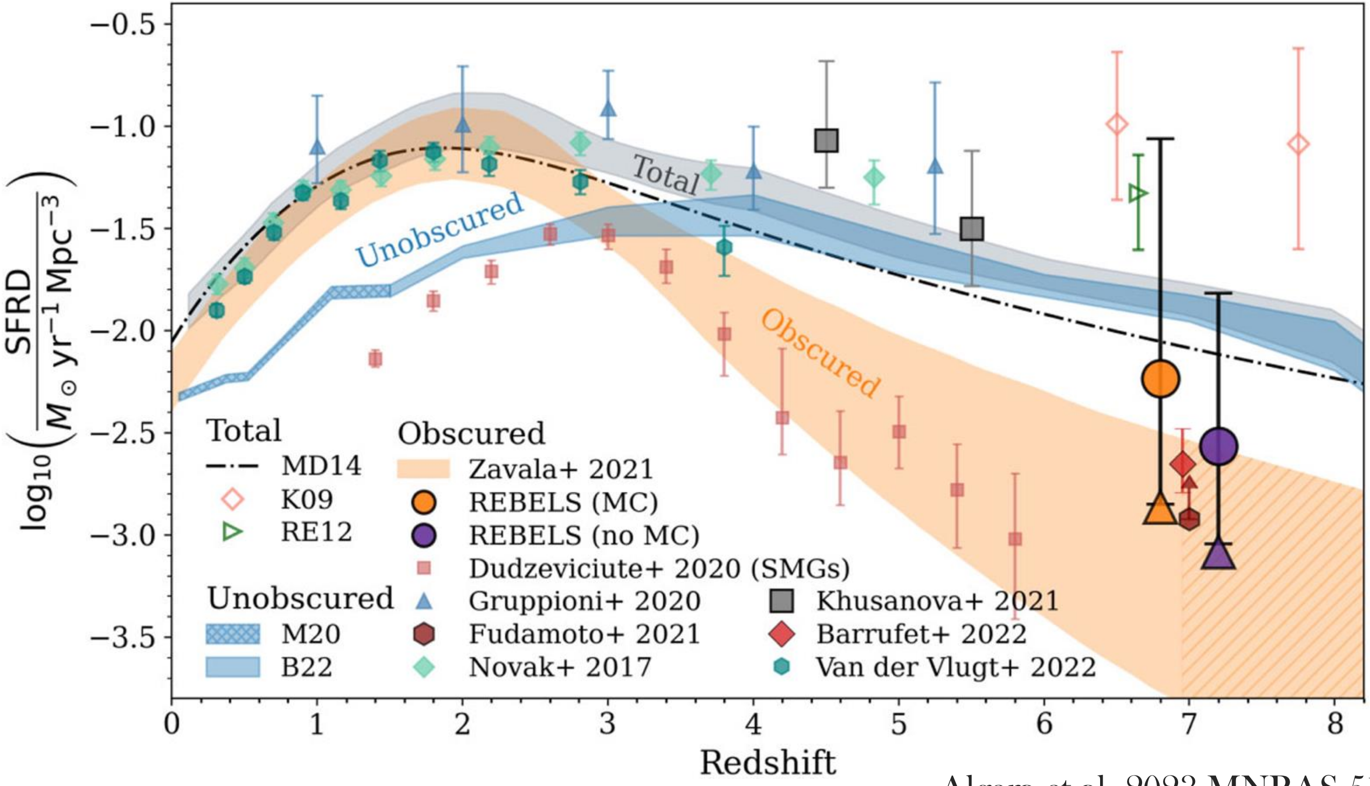
Modelling Cosmic Dust Atom-by-Atom in a Multiphase ISM

Clarke Esmerian |Postdoc, "Origin and Fate of Dust in Our Universe" Wallenberg Collaboration |
Department of Space, Earth, and Environment | Chalmers University of Technology |
Heidelberg "Quo Vadis Galaxy Evolution?"

Cosmic Dust: Why Should We Care?

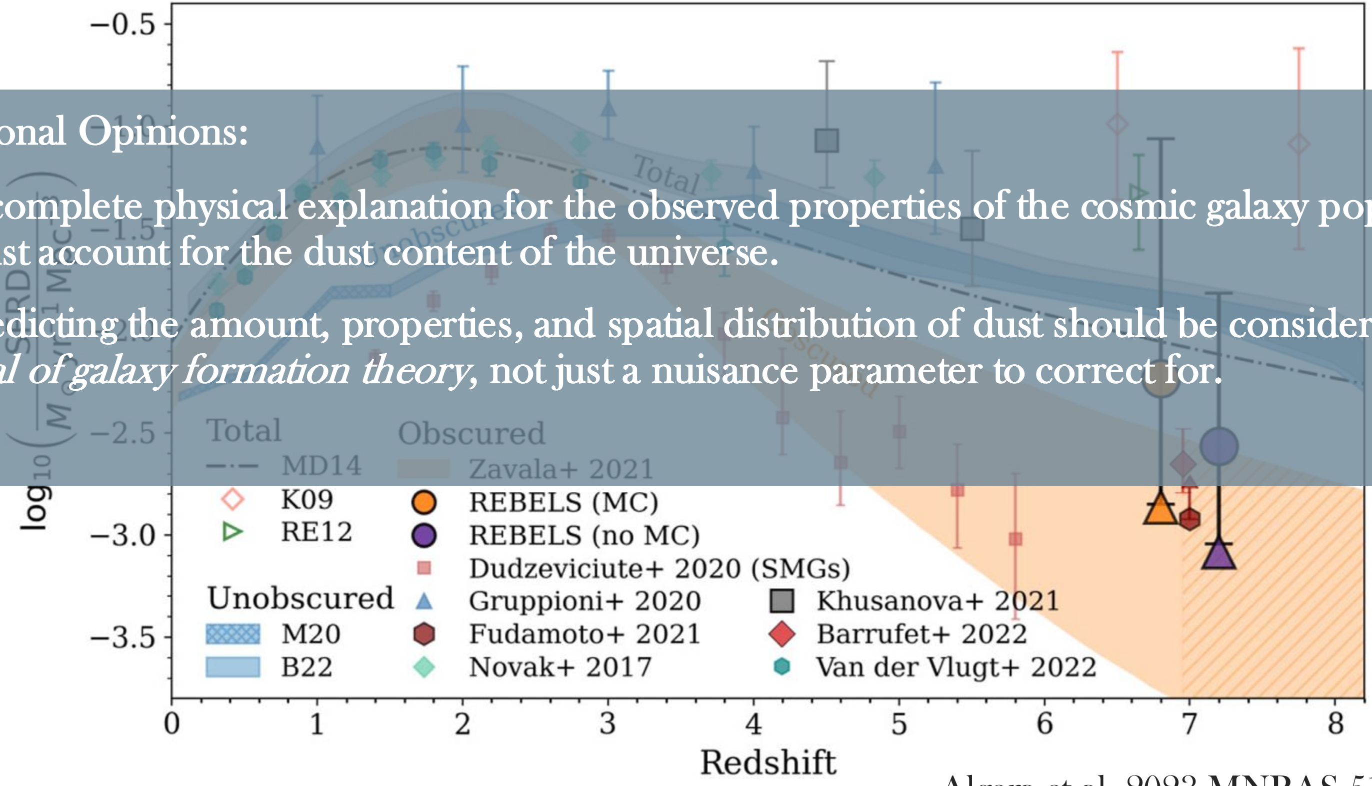
Well, it's everywhere!



Algera et al. 2023 MNRAS 518, 6142

Cosmic Dust: Why Should We Care?

Well, it's everywhere!



Personal Opinions:

- A complete physical explanation for the observed properties of the cosmic galaxy population must account for the dust content of the universe.
- Predicting the amount, properties, and spatial distribution of dust should be considered *a central goal of galaxy formation theory*, not just a nuisance parameter to correct for.

Algera et al. 2023 MNRAS 518, 6142

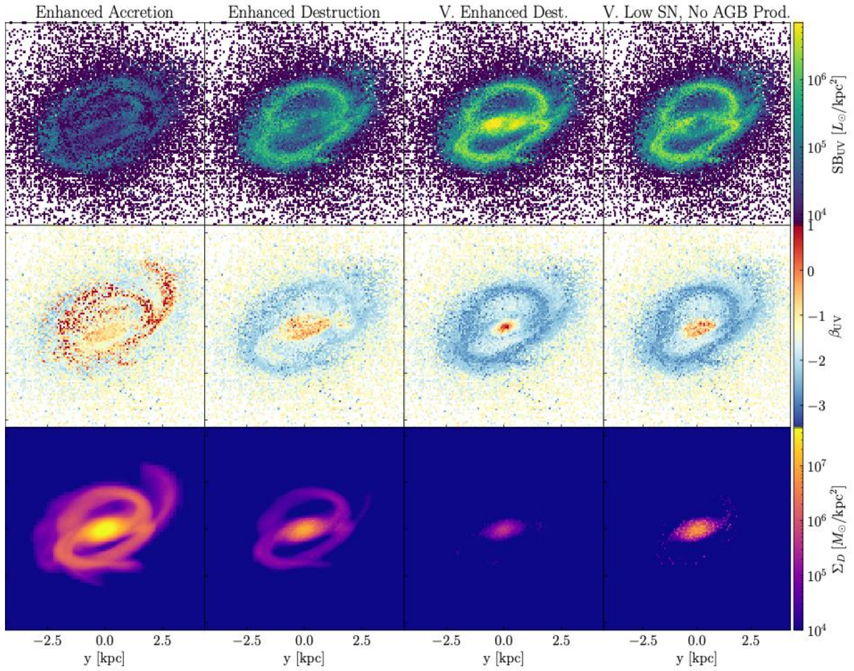
Dust Physics: Important but Uncertain

- The properties of dust are non-uniform and evolving
- Multiple processes determine its amount and material properties, but they remain incompletely understood
  - Nucleation: Supernovae Remnants, AGB, Wolf-Rayet, ...
  - Gas-Grain Transfer
    - Growth via Gas-Phase Accretion
    - Sublimation & Photodesorption
    - Thermal & Non-thermal Sputtering
  - Grain-grain collisions
    - Coagulation
    - Shattering
    - Vaporization
  - Shocks (combination of all above)

A complete physical understanding of the cosmic dust lifecycle will ultimately require the accounting for all of these processes and their interaction in a turbulent, multiphase ISM.

Dust Physics: Important but Uncertain

Example: Parameter Exploration with a simple Dust Model + CROC Simulations



Esmerian & Gnedin 2022 ApJ 940, 74
Esmerian & Gnedin 2024 ApJ 968, 113

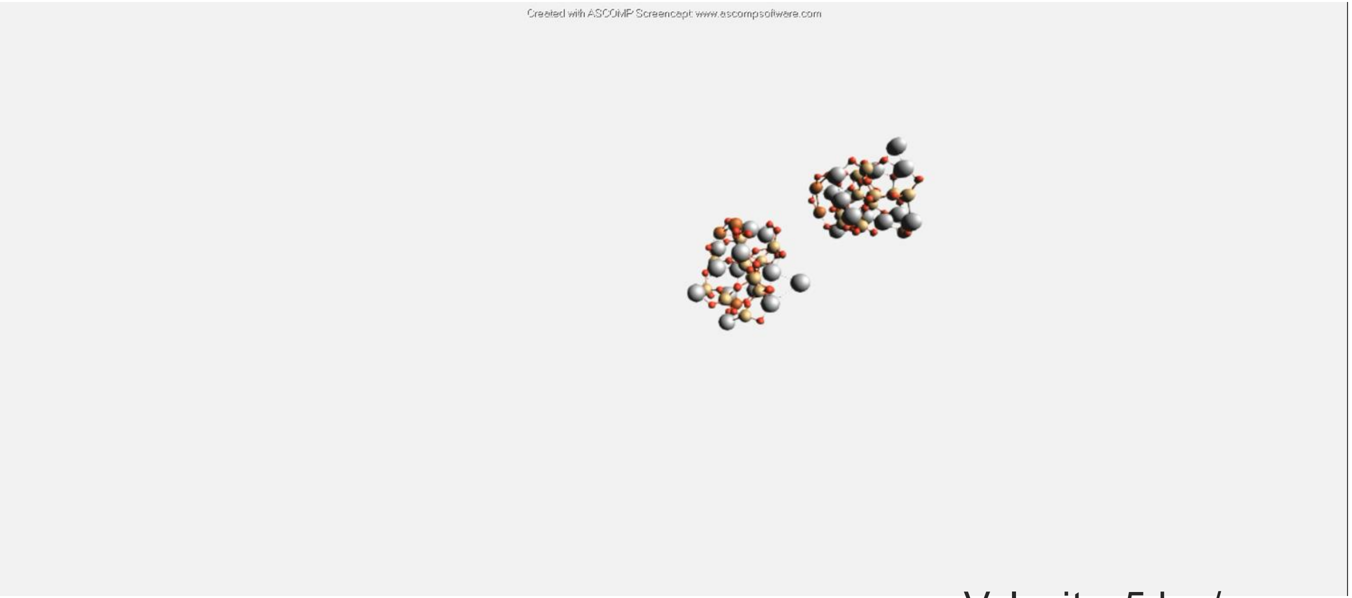
- Simulations from the Cosmic Reionization On Computers (CROC) project (Gnedin 2014, 2017)
- Dust model based on Feldmann 2015. Evolved on tracer particles in post-processing.
- Different reasonable choices for dust physics parameters give vastly different predictions for amount and spatial distribution of dust
- Uncertainties in dust physics are coupled to uncertainties in ISM physics…what are we to do?

One Approach: Molecular Dynamics

Methods

- Unlike many atomic/ionic processes in the ISM, dust physics processes are many-body problems and usually must be characterized numerically or empirically
- (closer to) First-principles estimates for some of these processes are possible with *molecular dynamics simulations*

PRELIMINARY



Velocity: 5 km/s

PRELIMINARY

One Approach: Molecular Dynamics

Methods

- Full Schrödinger-equation solutions are too computationally expensive, two levels of approximation:
  - **Density Function Theory (DFT)** is a fully quantum-mechanical method based on the electron density field, as opposed to the full many-body wavefunction, which is mapped onto the total energy (a *functional* of the *density*), which then determines dynamics
    - Accurate but expensive: use for calculating initial molecular structures, binding energies

  - **Reactive Force Field (ReaxFF)** evolves the dynamics classically with parameterized, empirically-calibrated bond-order-dependent potentials to simulate chemical reactions by allowing bonds to form and break during simulations.
    - Less accurate but cheaper: use for more complicated and rapidly evolving dynamics such as collisions

Dust Physics: Important but Uncertain

CHALMERS
UNIVERSITY OF TECHNOLOGY

- Multiple processes determine its amount and material properties, but they remain incompletely understood
  - Nucleation: SNR, AGB, WR, …
  - Gas-Grain Transfer
    - Growth via Gas-Phase Accretion (amorphous carbon)
    - Sublimation & Photodesorption
    - Thermal & Non-thermal Sputtering
  - Grain-grain collisions (amorphous carbon and "astrodust" silicates)
    - Coagulation
    - Shattering
    - Vaporization
  - Shocks (combination of all above)

A complete physical understanding of the cosmic dust lifecycle will ultimately require the accounting for all of these processes and their interaction in a turbulent, multiphase ISM.

Gas-Phase Accretion

Background

Growth rate for an individual dust grain of species s mass m_s, temperature T_s and (effective) grain size a_s

$$\frac{dm_s}{dt} = \sum_i m_i n_i \langle \sigma_{s,i} v_i \rangle = a_s^2 \sum_i \alpha_{s,i} n_i \left(8\pi m_i k_B T_g\right)^{1/2}$$

where i enumerates gas-phase species with particle masses m_i, gas temperature T_g, and number density n_i, and $\alpha_{s,i}$ is the thermal-velocity-averaged **sticking coefficient**

$$\alpha_{s,i}(T_g, T_s) \equiv \int_{T_g} dv_i S_{s,i}(v_i, T_s) v_i f(v_i)$$

which is dependent on the velocity- and species-dependent sticking probability $S_{si}(v_i)$.

Gas-Phase Accretion

Background

For OOM estimation, approximate as

$$\frac{dm_s}{dt} \approx \langle\alpha\rangle a_s^2 Z n_g \left(8\pi\mu_Z m_H k_B T_g\right)^{1/2}$$

and to get mass-growth timescale,

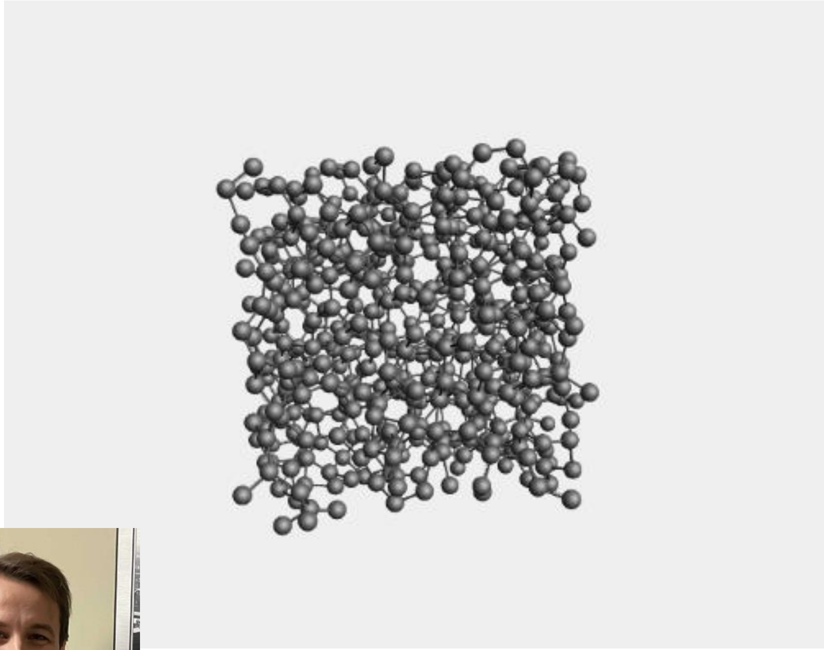
$$\tau \approx \frac{m_s}{\frac{dm_s}{dt}} \approx \left(\frac{\pi}{8\mu_Z m_H}\right)^{\frac{1}{2}} \langle\alpha\rangle^{-1} a_s \rho_s \left(Z n_g\right)^{-1} \left(k_B T_g\right)^{-1/2}$$

Factoring out the sticking coefficients and assuming $\mu_Z = 20$, $a_s = 0.1\mu\text{m}$, $\rho_s = 3\ g\ cm^{-3}$, $Z = 0.5Z_\odot = 0.01$, then $\boldsymbol{\tau \approx O(Myr)}$ **for the dense molecular phase (**$\boldsymbol{n_g \approx 10^3 cm^{-3}, T_g \approx 10K}$**), "diffuse" molecular phase (**$\boldsymbol{n_g \approx 100 cm^{-3}, T_g \approx 50K}$**), and the cold neutral medium (**$\boldsymbol{n_g \approx 30 cm^{-3}, T_g \approx 100K}$**), and** $\boldsymbol{\tau \approx O(10\ Myr)}$ **in the warm neutral medium (**$\boldsymbol{n_g \approx 0.6\ cm^{-3}}$**,** $\boldsymbol{T_g \approx 5000K}$**).**

If sticking coefficients are order 0.1 or larger, ***grain growth happens on timescales comparable to or shorter than the lifetimes of molecular clouds.***

Gas-Phase Accretion

Sticking Coefficients for Carbonaceous Dust

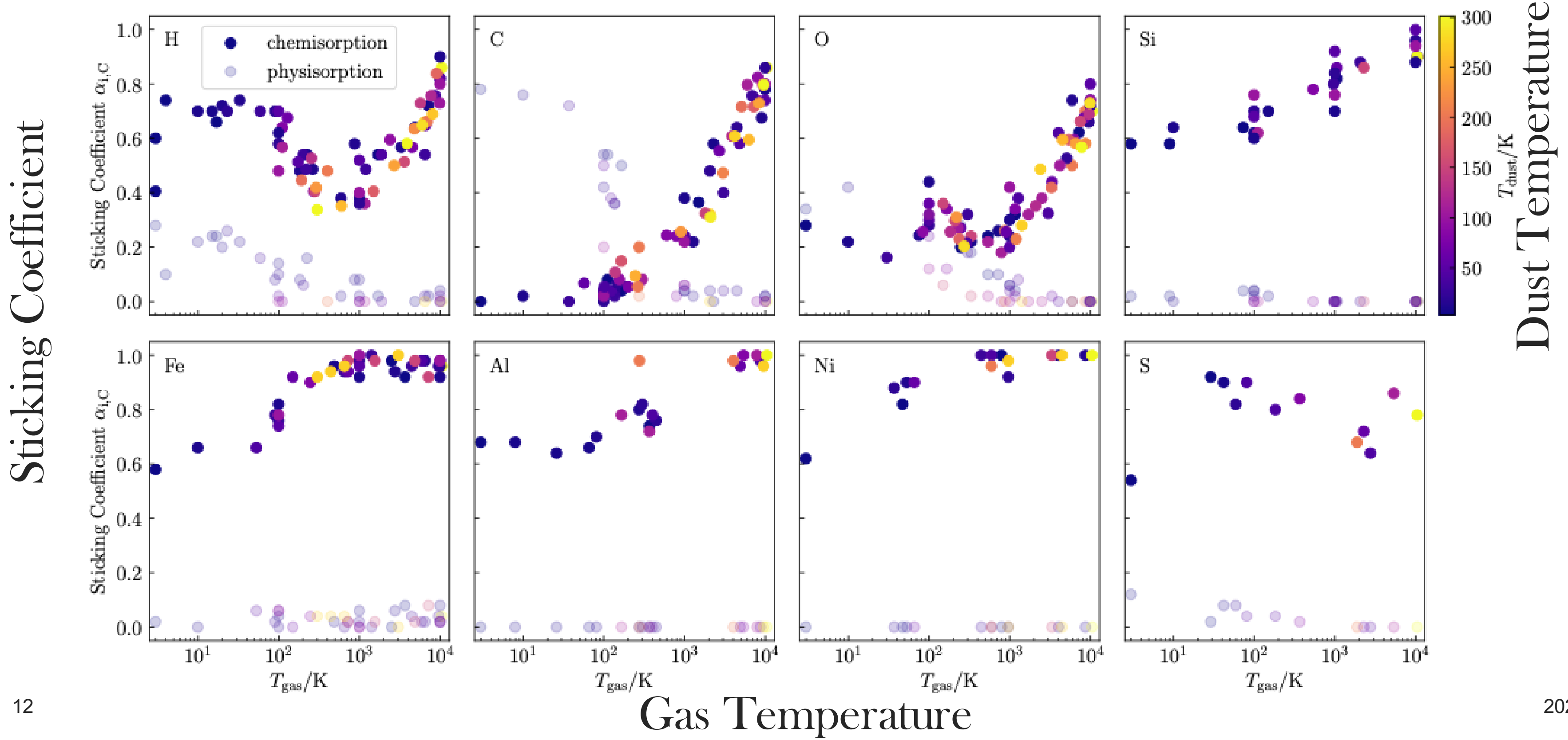


Duncan Bossion, University of Rennes

- 20Å-side square of amorphized *pure* amorphous carbon (a-C), representing surfaces of larger grain
- Throw atoms, see if they stick
- Building on Bossion et al. 2024 (A&A, 692, A249), which first did this assuming same grain and gas temperature – relevant for dense environments in which grains nucleate.
- Re-calculated for ISM conditions:
  - Gas temperatures: 3-10^4 K
  - Grain temperatures: 3-300 K
- Train a neural network to interpolate between sampled temperatures & predict for additional elements (in progress)

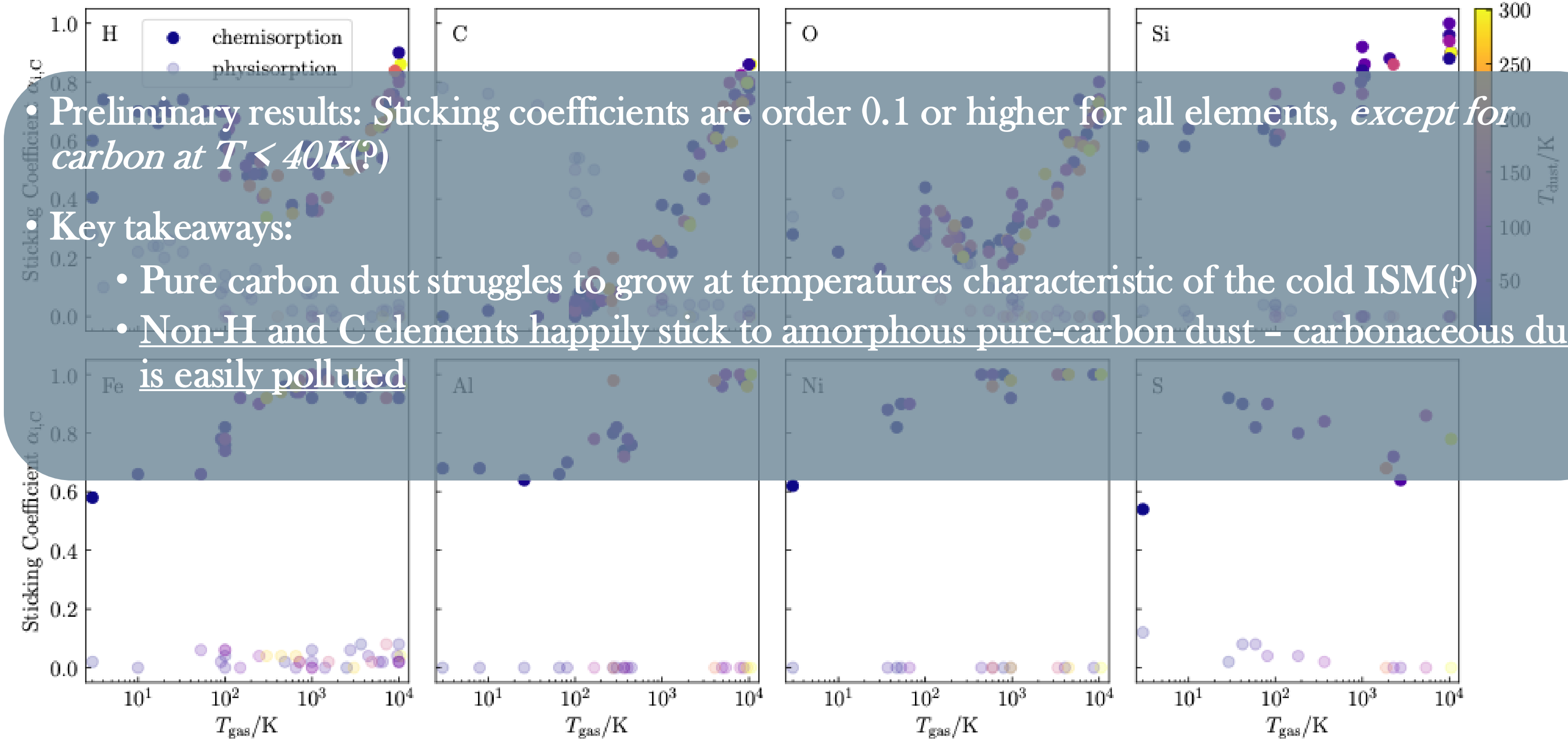
Gas-Phase Accretion

Sticking Coefficients for Carbonaceous Dust



Gas-Phase Accretion

Sticking Coefficients for Carbonaceous Dust



- Preliminary results: Sticking coefficients are order 0.1 or higher for all elements, *except for carbon at T < 40K*(?)
- Key takeaways:
  - Pure carbon dust struggles to grow at temperatures characteristic of the cold ISM(?)
  - <u>Non-H and C elements happily stick to amorphous pure-carbon dust – carbonaceous dust is easily polluted</u>

Gas-Phase Accretion

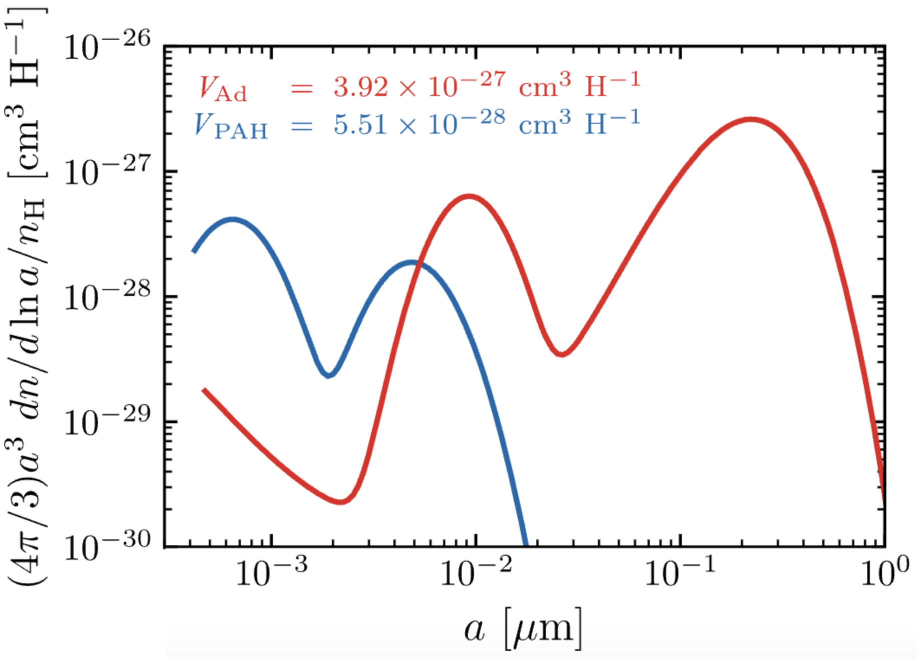
Sticking Coefficients for Carbonaceous Dust

- Consequences: ***Do we need to reconsider the two population carbonaceous-silicate paradigm?***
  - Well-motivated in nucleation environments (SNR, AGB): CO formation is the fastest process, C/O ratio determines remaining gas-phase abundances.
  - Even Hensley & Draine 2021, 2023 assume composite "Astrodust" particles with separate carbonaceous and silicate inclusions. THEMIS (Jones 2017, Ysard 2024) has silicate cores, carbon mantels.
  - Might need to consider a much larger set of material compositions, optical properties, molecular dynamics initial conditions …

- Much more to do:
  - Sticking coefficients for remaining abundant elements – neural network
  - *Hydro*carbons
  - Silicates
  - Effects of Ice Mantels, Sublimation & Desorption (binding energy distributions)

Grain-Grain Collisions

Background



Hensley & Draine 2023, ApJ 948, 55

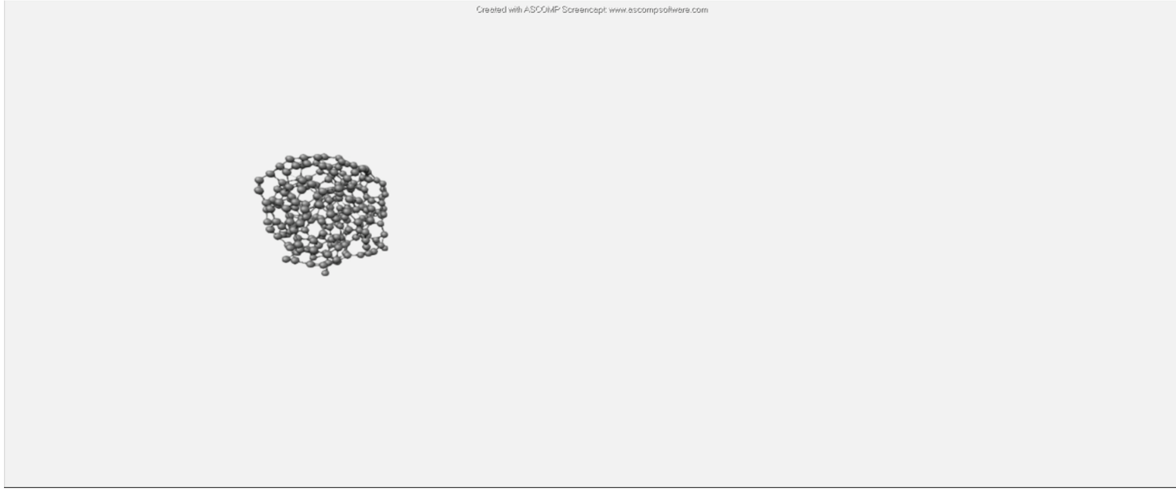
- Grains can collide with each other, and the outcome depends on their relative velocities
  - Coagulation: stick together
  - Shattering: break apart
  - Vaporization: return to gas phase
- Traditionally assumed velocity thresholds:
  - Shattering: 1.2 km/s for Carbon, 2.7 km/s for Silicate (Jones, Tielens, & Hollenbach, 1996)
  - Vaporization: 23 km/s for Carbon, 19 km/s for Silicate (Tielens et al. 1994)
- Timescale: $v \approx 1 - 10\ km/s$ (Yan, Lazarian, & Hirashita 2004) $\tau \sim n\sigma v$
  - Dense Molecular: $O(1\ Myr)$
  - "Diffuse" Molecular: $O(10\ Myr)$
  - CNM: $O(10\ Myr)$
  - WNM: $O(100\ Myr)$

Grain-Grain Collisions

Amorphous Pure Carbon

Molecular Dynamics Simulations:

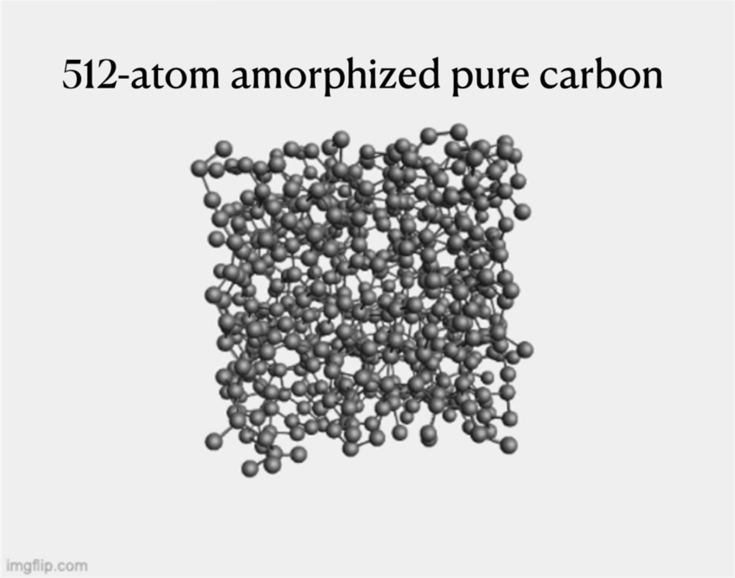
- "Molecule Gun" simulations
- Classical Dynamics + ReaxFF (Reactive Force Field) Potentials
- Time evolution: 0.25 fs * 50000 steps = 12500 fs = 1.25×10^{-11}s
- Materials: amorphous pure carbon
- Grain shapes: spherical, non-porous
- Velocities: 0.001 km/s to 20 km/s
- Initial Grain Temperature: 10K



Grain-Grain Collisions

Amorphous Pure Carbon: Grain "Construction"

Bossion et al. 2024 (A&A, 692, A249)



Cut → Smaller grains of 64, 125, 210, 420 atoms (~7, 10, 12, 16 Å)

↓ Collision

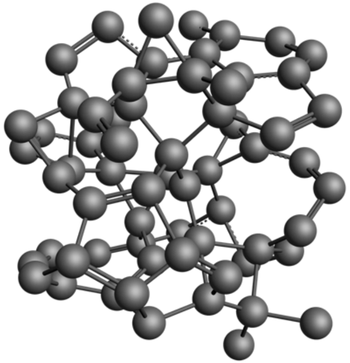
Larger grains

↓ Thermalized

~24-52 Å

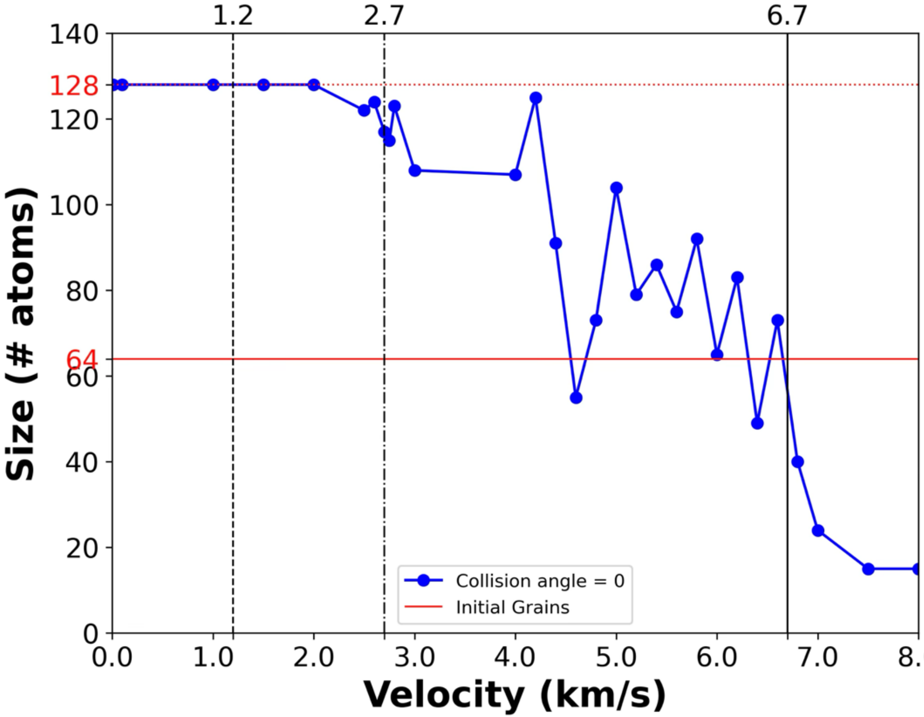
Grain-Grain Collisions

Amorphous Pure Carbon: Results – Small Clusters



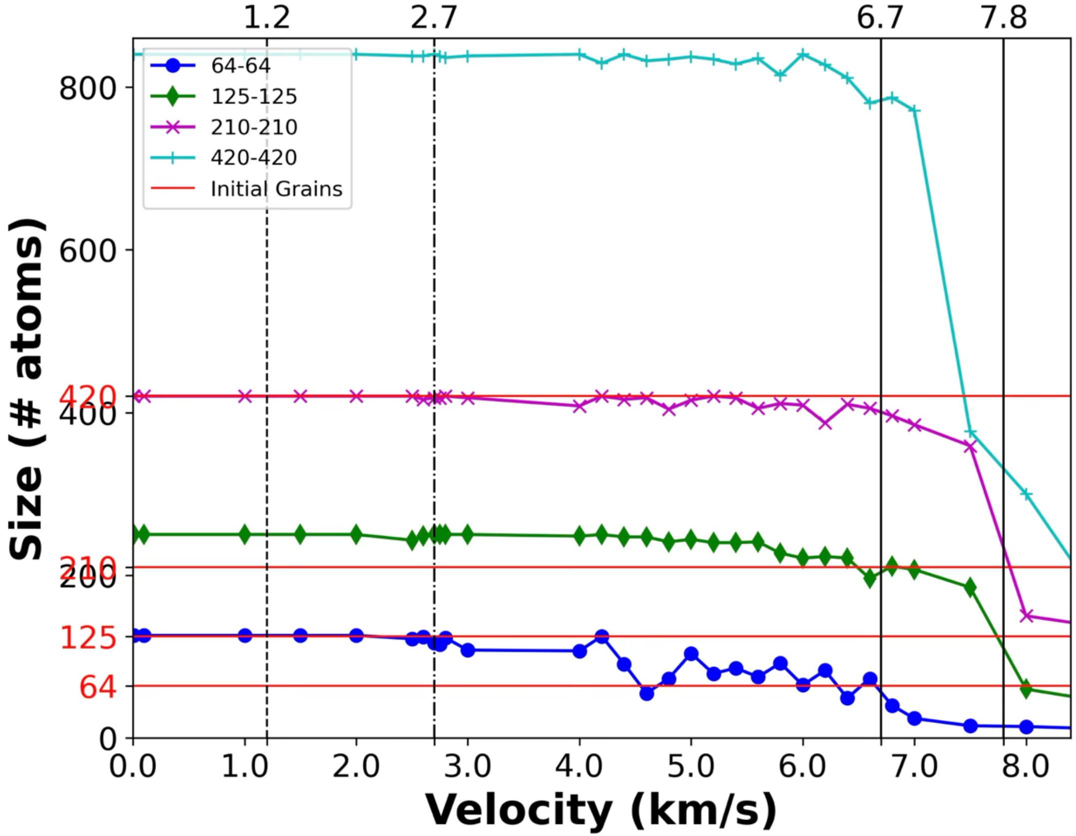
64 Atoms

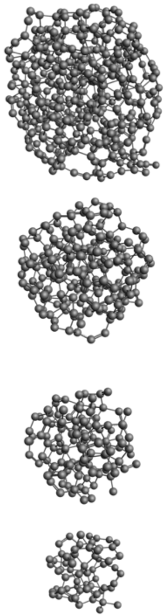
~ 7 Å



Grain-Grain Collisions

Amorphous Pure Carbon: Results – Larger Grains





Grain-Grain Collisions

"Astrodust" Silicates: Cluster Construction

THE ASTROPHYSICAL JOURNAL, 909:94 (21pp), 2021 March 1 https://doi.org/10.3847/1538-4357/abd6c6

CrossMark

The Dielectric Function of "Astrodust" and Predictions for Polarization in the 3.4 and 10 μm Features

B. T. Draine and Brandon S. Hensley[1]
Department of Astrophysical Sciences, Princeton University, Princeton, NJ 08544-1001, USA; bhensley@astro.princeton.edu, draine@astro.princeton.edu
Received 2020 September 22; revised 2020 December 21; accepted 2020 December 22; published 2021 March 9

Abstract

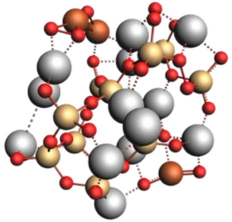
The dielectric function of interstellar dust material is modeled using observations of extinction and polarization in the infrared, together with estimates for the mass of interstellar dust. The "astrodust" material is assumed to be a mix of amorphous silicates and other materials, including hydrocarbons producing an absorption feature at 3.4 μm. The detailed shape of the 10 μm polarization profile depends on the assumed porosity and grain shape, but the 10 μm spectropolarimetric data are not yet good enough to clearly favor one shape over another, nor to constrain the porosity. The expected 3.4 μm feature polarization is consistent with existing upper limits, provided the 3.4 μm absorption is preferentially located in grain surface layers; a separate population of non-aligned carbonaceous

Nominal Composition of Astrodust Grains

f_{Fe} =	0	0.10
Species	(ppm relative to H)	
$Mg_{1.3}(Fe,Ni)_{0.3}SiO_{3.6}$ ($\rho = 3.41$ g cm^{-3})	35.4	35.4
(Fe,Ni) metal ($\rho = 7.9$ g cm^{-3})	0	4.5
$(Fe,Ni)_3O_4$ ($\rho = 5.15$ g cm^{-3})	8.9	7.4
(Fe,Ni)S ($\rho = 4.84$ g cm^{-3})	7.6	7.6
$CaCO_3$ ($\rho = 2.71$ g cm^{-3})	3.2	3.2
Al_2O_3 ($\rho = 4.02$ g cm^{-3})	1.7	1.7
SiO_2 ($\rho = 2.20$ g cm^{-3})	2.8	2.8
C (in hydrocarbons, $\rho \approx 2$ g cm^{-3})	83.	83.
C in PAH nanoparticles	40.	40.

62 Atoms

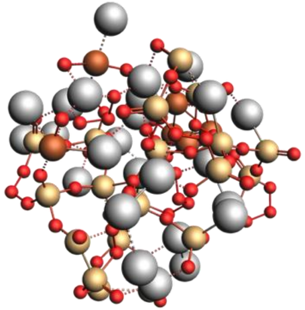
8 Å



$(Mg_{13}Fe_3Si_{10}O_{36})_2$

124 Atoms

13 Å



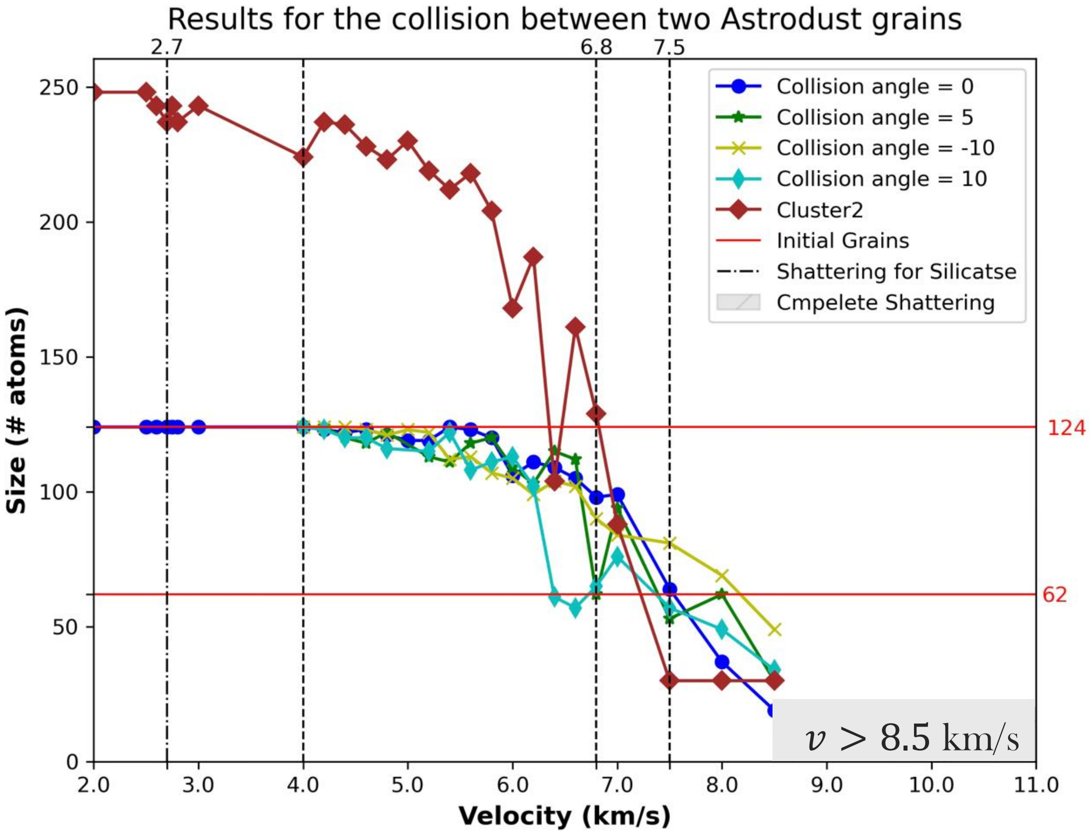
W. M. C. Sameera, University of Gothenburg

Grain-Grain Collisions

“Astrodust” Silicates: Results

Grain-Grain Collisions

“Astrodust” Silicates: Results

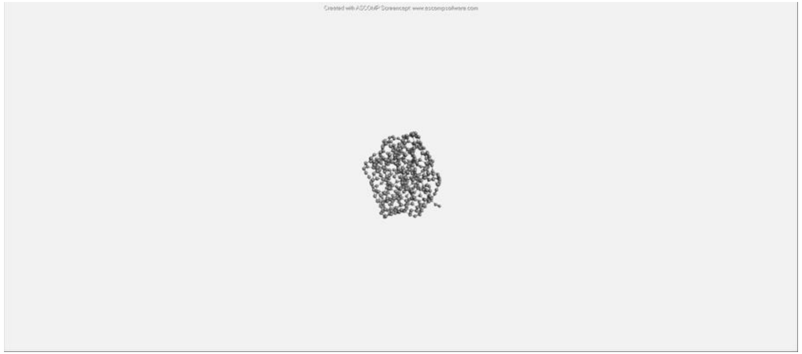


Grain-Grain Collisions

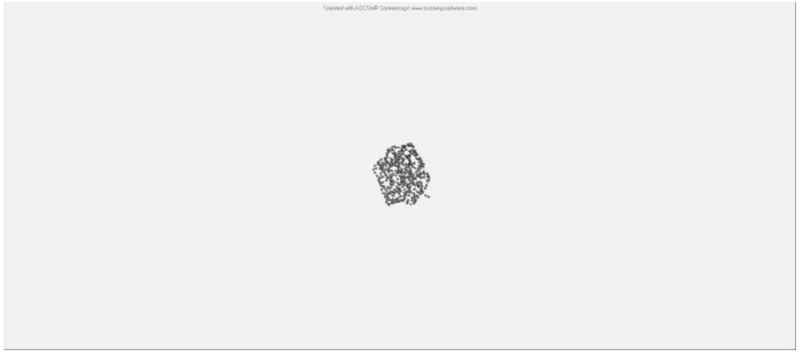
“Astrodust” Silicates: Results

Grain-Grain Collisions

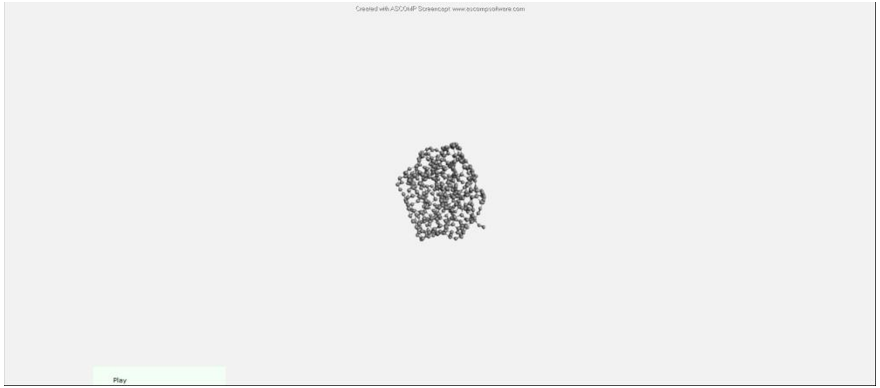
Composite Grain Formation? Apparently Not!: SiO_2 + Amorphous carbon



PRELIMINARY



PRELIMINARY



PRELIMINARY

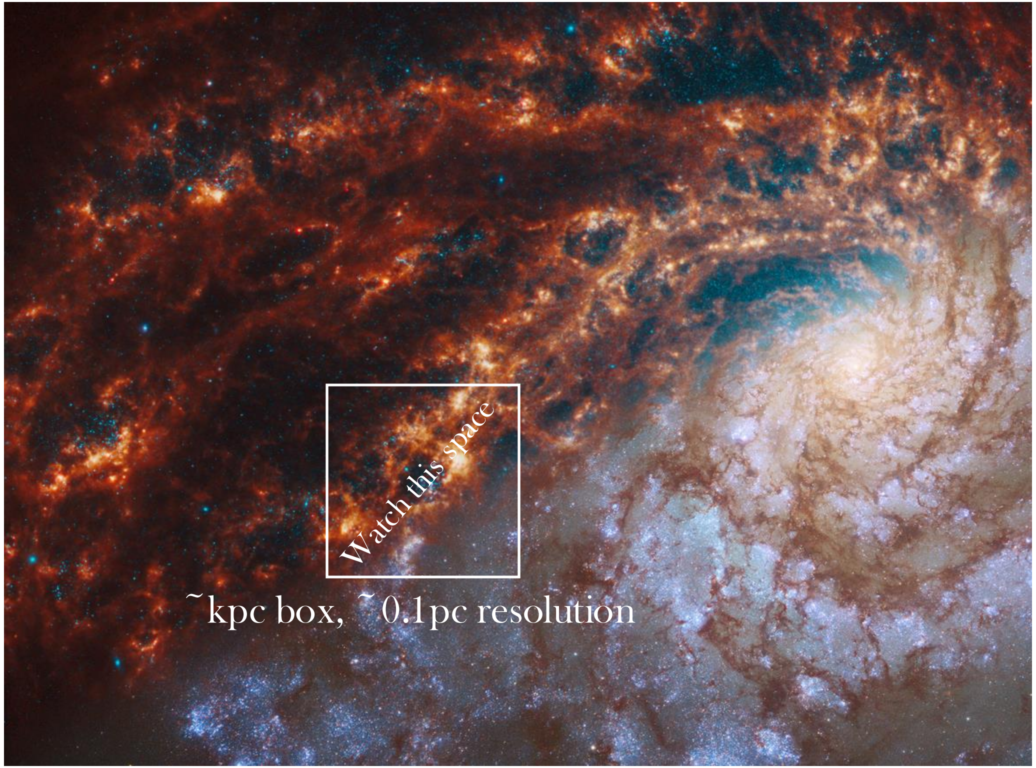
Grain-Grain Collisions

Summary

- Preliminarily, the classic Jones et al. 1996 shattering thresholds of 1.2 km/s and 2.7 km/s for carbonaceous and silicate materials may be an underestimate, for some materials by a factor of 2 or larger, at least for smaller (< 60Å) grains.
- However, the *vaporization* threshold at which most of the material is returned to the gas phase appears to be *smaller* than the traditionally assumed values (Tielens et al. 1994) by similar factors, again for these small grains.
- Collisions between SiO_2 and amorphous carbon clusters don't stick – fail to form larger grains of composite material
- *Much* more to do:
  - Uncertainties in molecular dynamics methods: check with DFT. Empirical data…?
  - Analyze shattered grain size distributions
  - *Hydro*carbons, more materials, ice mantles, "polluted grains"
  - Grain thermal history

Quo Vadis? Putting it All Together in a Multiphase ISM

Kpc-Scale Fluid-Dynamical Simulations of a Galactic Disk Patch



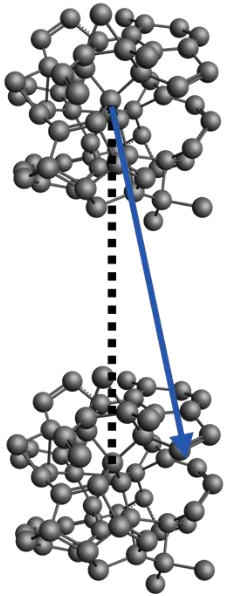
NASA, ESA, CSA, STScI, Janice Lee (STScI), Thomas Williams (Oxford), PHANGS Team

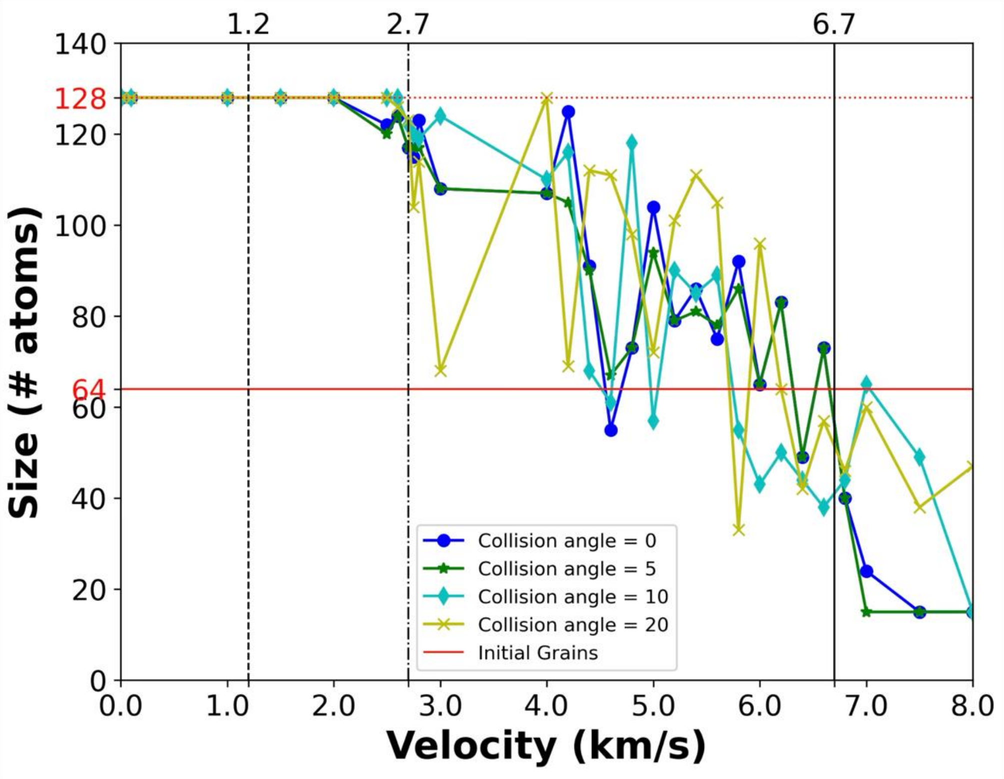
Thanks!

CHALMERS
UNIVERSITY OF TECHNOLOGY

Grain-Grain Collisions

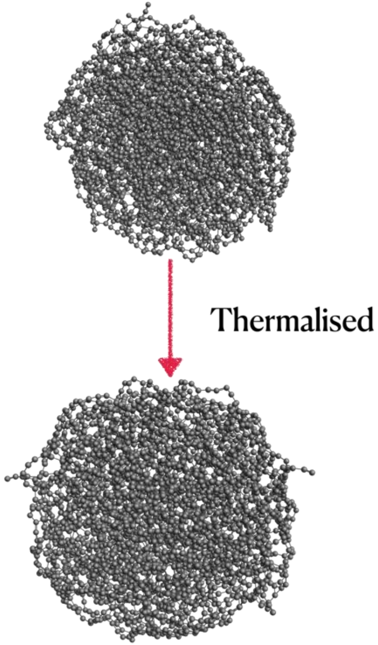
Amorphous Pure Carbon: Results – Impact Angle





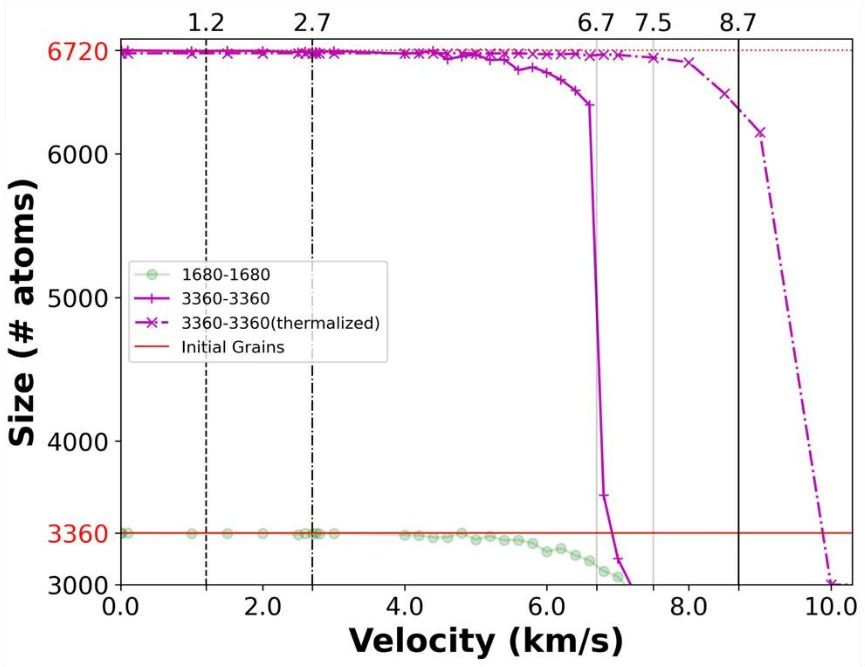
Grain-Grain Collisions

Amorphous Pure Carbon: Results – Larger Grains



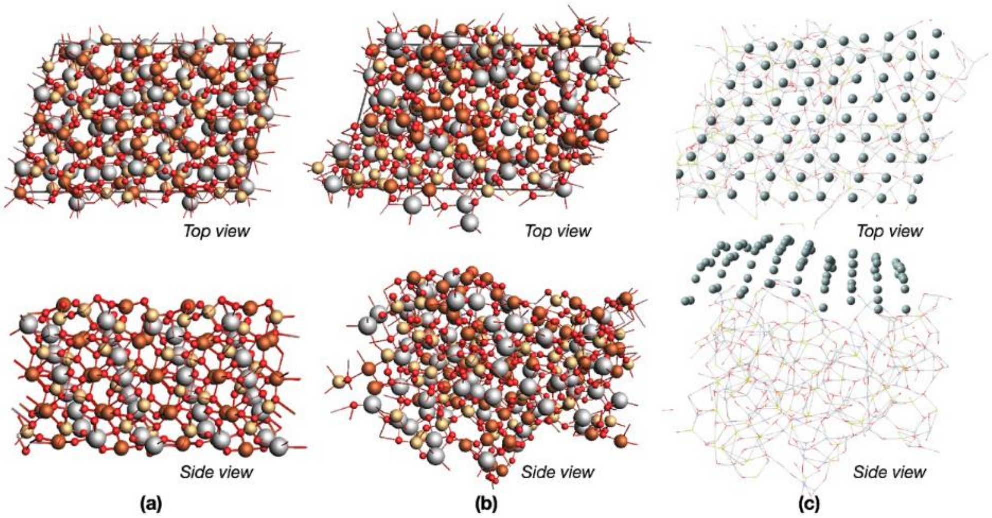
3360 Atoms

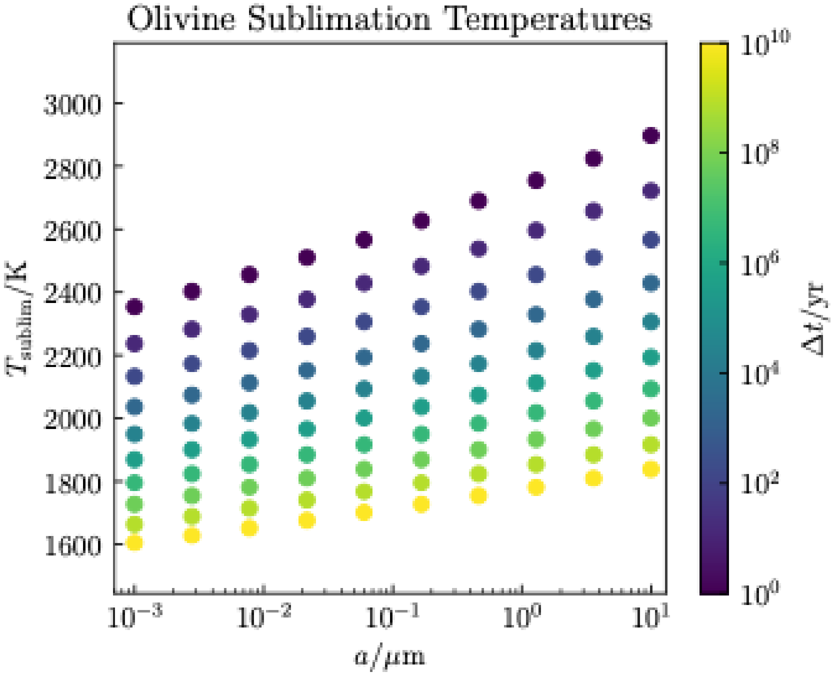
Thermal History?



Sublimation and Desorption: Binding Energies

$FeMgSiO_4$ Silicate Slabs





Kristoffer Hansson, W. M. C. Sameera