A Comparative Analysis of Gemstones for Laser Applications based on Digital and Simulation Methods

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ABSTRACT

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BACKGROUND

Laser applications of gemstones

METHOD

Digital microscopic and simulation methods

AIM

A comparative analysis of sapphire, ruby, and diamond crystals

RESULTS AND CONCLUSION

Enhancing the properties of the precious stones and improving the laser technologies in which they are implemented.

ACCENTS IN THE INTRODUCTION

- **FEMTOSECOND LASERS**
  - titanium-doped sapphire crystal is suitable for integration into innovative 3D printing technologies due to the wider bandwidth of laser emission compared to the semiconductor lasers commonly used in 3D printers.

- **DIODE LASERS**
  - CVD (Chemical Vapor Deposition) diamond is a boron-doped structure that can be implemented in semiconductors in order to improve their characteristics for implementation in 3D printers.

Advantages of Using Sapphire Crystals

- A higher level of optical transparency in determined spectral regions is crucial for the proper functioning of the femtosecond lasers, as they utilize various types of light radiation that must effectively pass through these regions.

Advantages of Using Diamond Semiconductors

- Enhancing the accuracy and resolution of printing due to the faster electronics.
- Due to the excellent thermal conductivity and electrical conductivity achieved through the boron doping, power consumption and device heating can be reduced, providing a more efficient and economical additive process.
- The reliability of the machine increases thanks to the thermal, chemical, and mechanical stability ensured by the diamond components.

Content

Section II — Related work

- *A comparative characteristics of sapphire and ruby*
- *A comparative characteristics of sapphire and diamond for laser applications*

Section III — Assessment and Analysis of Results Generated from Simulation Modeling of Gemstones

A. Possible influence of impurities on the quality of laser radiation emission.

B. The impact of the bond type on the quality of laser radiation emission.

C. The influence of grain growth on the quality of laser emission.

II. Related Work

A comparative Characteristics of Sapphire and Ruby

Characteristics	Sapphire	Ruby
Group	corundum	corundum
Chemical formula	Al_2O_3	Al_2O_3
Bond type	ionic-covalent	ionic-covalent
Mohs Hardness	9	9
Impurities	Titanium (Ti)	Chromium (Cr)
Most common color	various shades of blue	red, violet-red hues
Excitation peak, nm	396	410
Emission peak, nm	511	670-710
Transparency	high	high
Conversion efficiency	high	medium to high

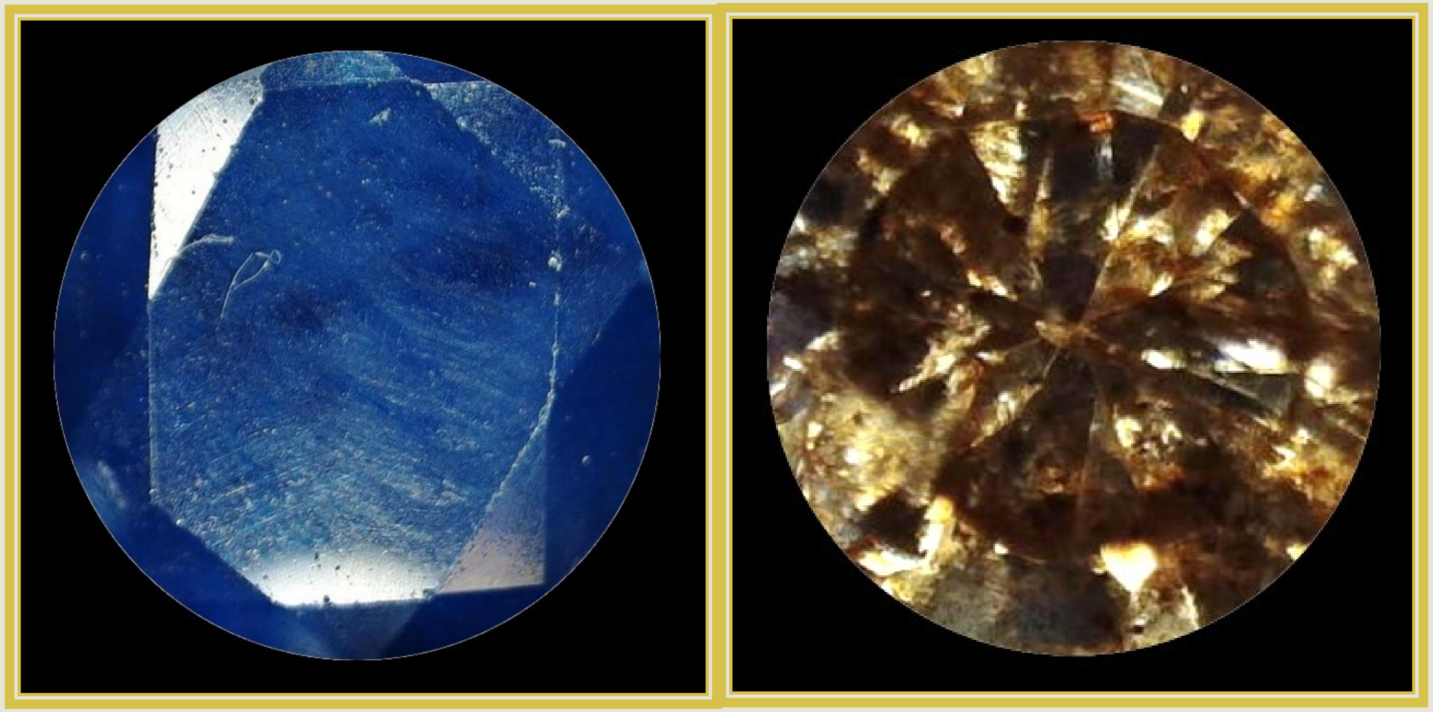
A comparative Characteristics of Sapphire and Diamond for Laser Applications

Characteristics	Doped sapphire	Diamond	Doped diamond
Bond type	ionic-covalent	strong covalent	strong covalent
Mohs Hardness	9	10	10
Optical properties	wide spectrum	visible light, IR spectrum	visible light, IR spectrum
Thermal conductivity	40 W/mK	2200 W/mK	> 2000 W/mK
Electrical conductivity	> 0	~ 0	> 0
Laser application	Femtosecond laser		Diode laser
Laser speed	very high, fs		high, ns
Laser doping materials	Titanium (Ti)	Not specified	Boron (B)
Laser precision	very high		high
Laser compactness	medium		very high

Possible Influence of Impurities on the Quality of Laser Radiation Emission

- In general impurities can cause energy losses and reduced laser efficiency due to possible unwanted absorption, refraction or scattering of light.

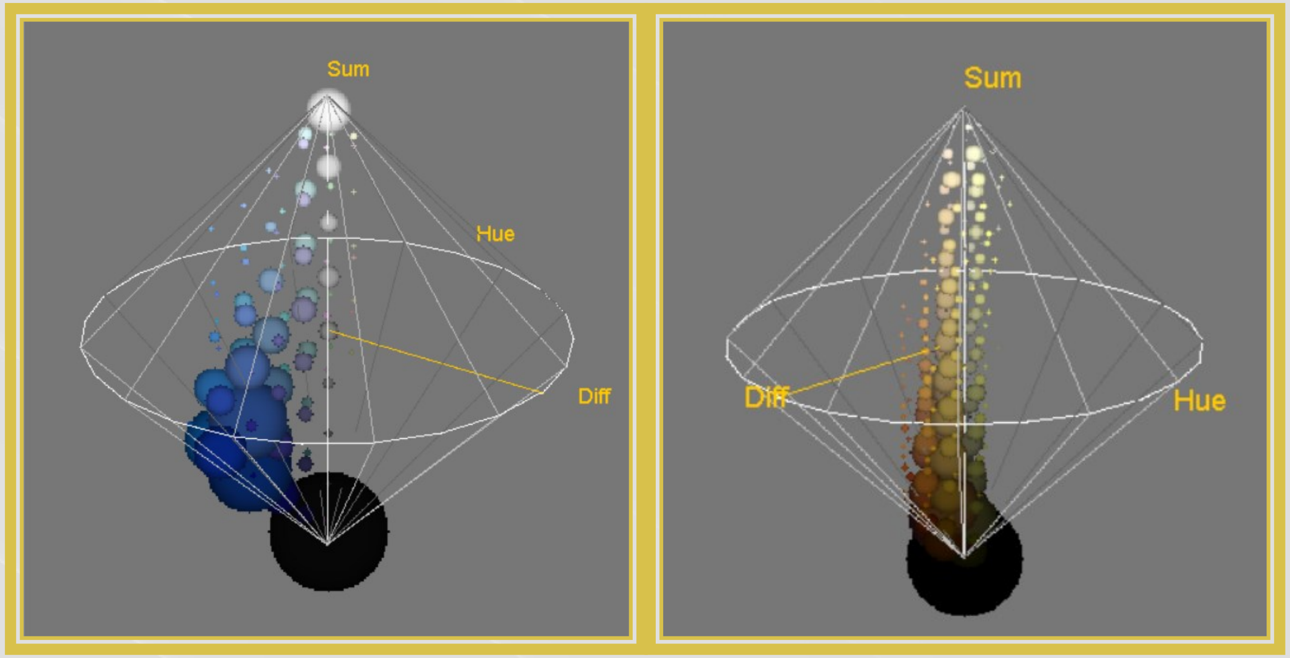
- Synthetic crystals are preferred for technical applications because of their high purity.



Microscopic images of a natural blue sapphire and a yellow diamond captured using a digital microscope Levenhuk DTX 90.

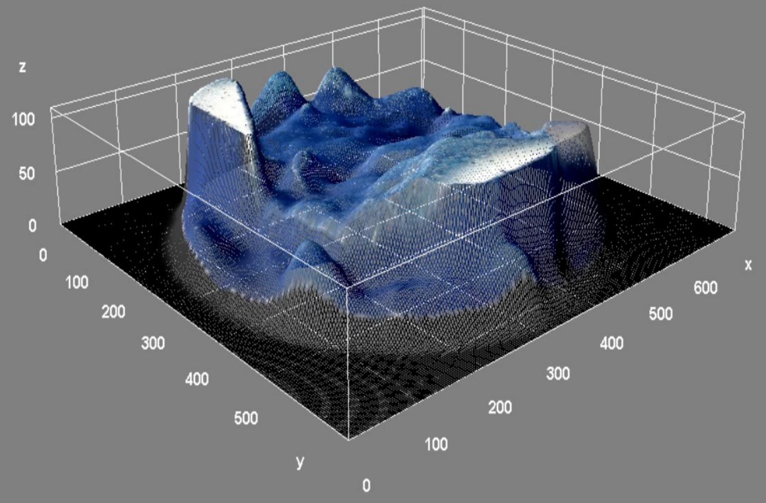
3D color profiling of gemstones for crystal analysis

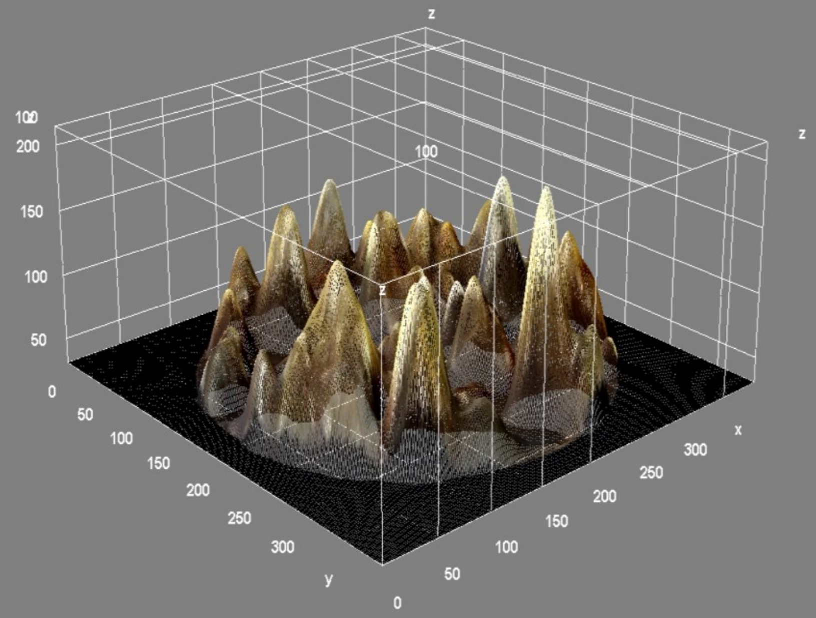
- The color gemstones are suitable for building very informative digital color profiles regarding the concentration and distribution of impurities in the crystal due to providing visual data for the color intensity and shape of the profiles.



3D color profiles of a sapphire and a diamond crystal, generated in Fiji.

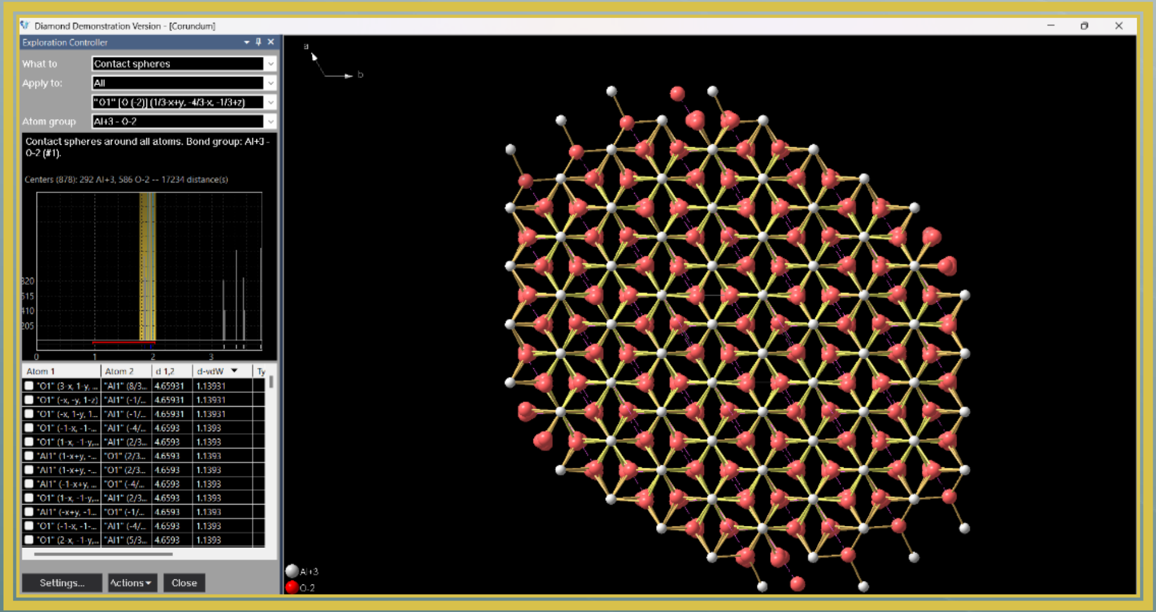
3D color profiles of a sapphire and a diamond crystal, generated in ImageJ



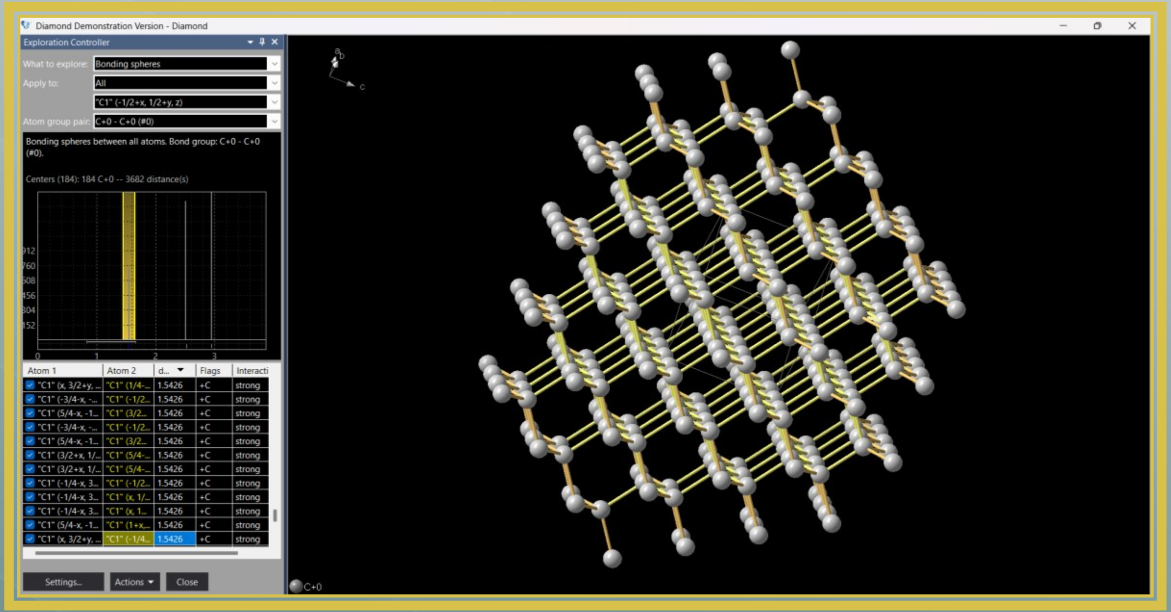


The Impact of the Bond Type on The Quality of Laser Radiation Emission

Crystal lattice interactions of a sapphire crystal at connecting groups Al+3 and O-2.



Crystal lattice interactions of a diamond crystal at connecting groups C+0 and C+0.



The visualizations of the crystal lattices of sapphire and diamond crystals are generated in the simulation software Diamond 5.

Assessment and Analysis of the Simulation Results

- In general, ionic and covalent bonds are strong, but covalent bonding is considered stronger than ionic bonding because the atoms share electrons around which a common electron shell is formed.
- In principle, the ionic-covalent bonds in the crystal lattice of sapphire can contribute to the stability of the laser and its high effectiveness, analogous to the role played by strong covalent bonds in the diamond crystal lattice.

The Influence of Grain Growth on the Quality of Laser Emission

Simulation Model (MaterialSim Grain Growth) from the Embedded Library of the Software NetLogo 6.4.0

Scenario I **The sapphire grains grow faster compared to the diamond grains**

- *In this case, a supposed impact could be greater dopant diffusion within the material, so that it is possible to enhance the efficiency of the laser emission.*

Scenario II **The diamond grains exhibit faster growth compared to the sapphire grains**

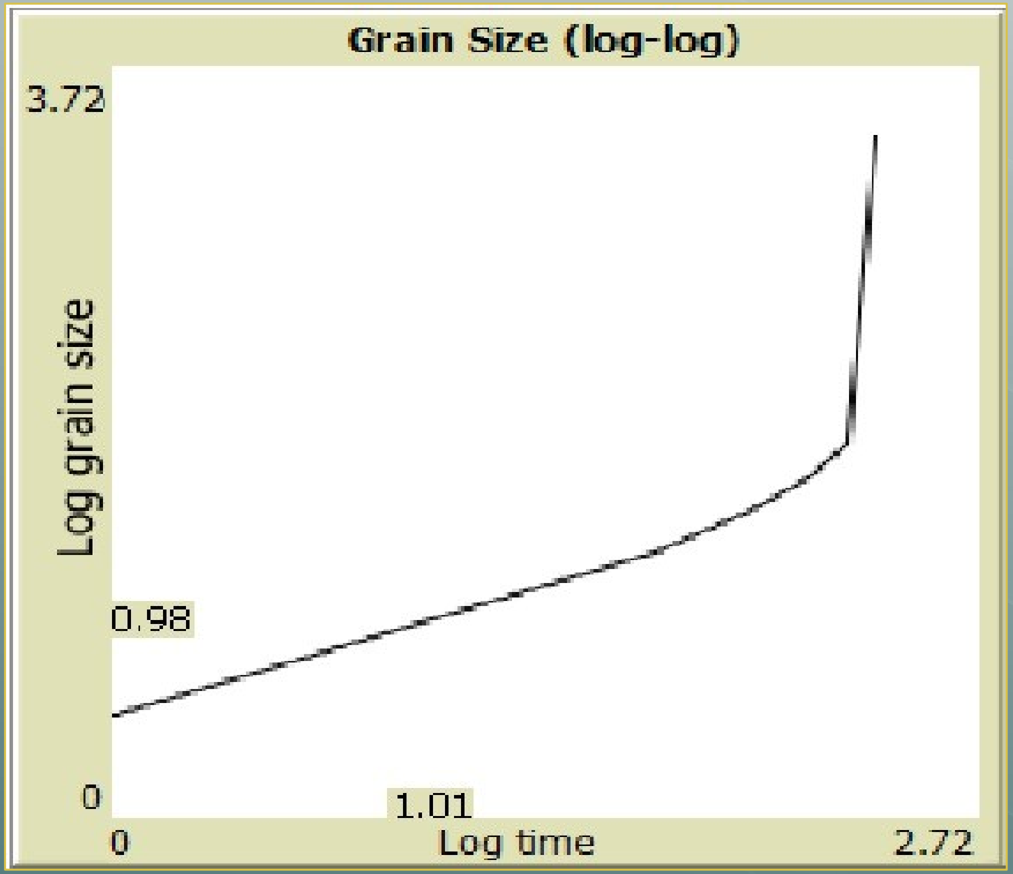
- *Firstly, achieving a denser crystal structure can enhance the coherence and stability of the laser.*
- *Furthermore, it can be observed that a more uniform distribution of impurities would optimize the laser performance.*
- *The faster increase in diamond grains could affect the thermal conductivity of the crystal and, in particular, its capability to dissipate heat generated during the laser working process.*

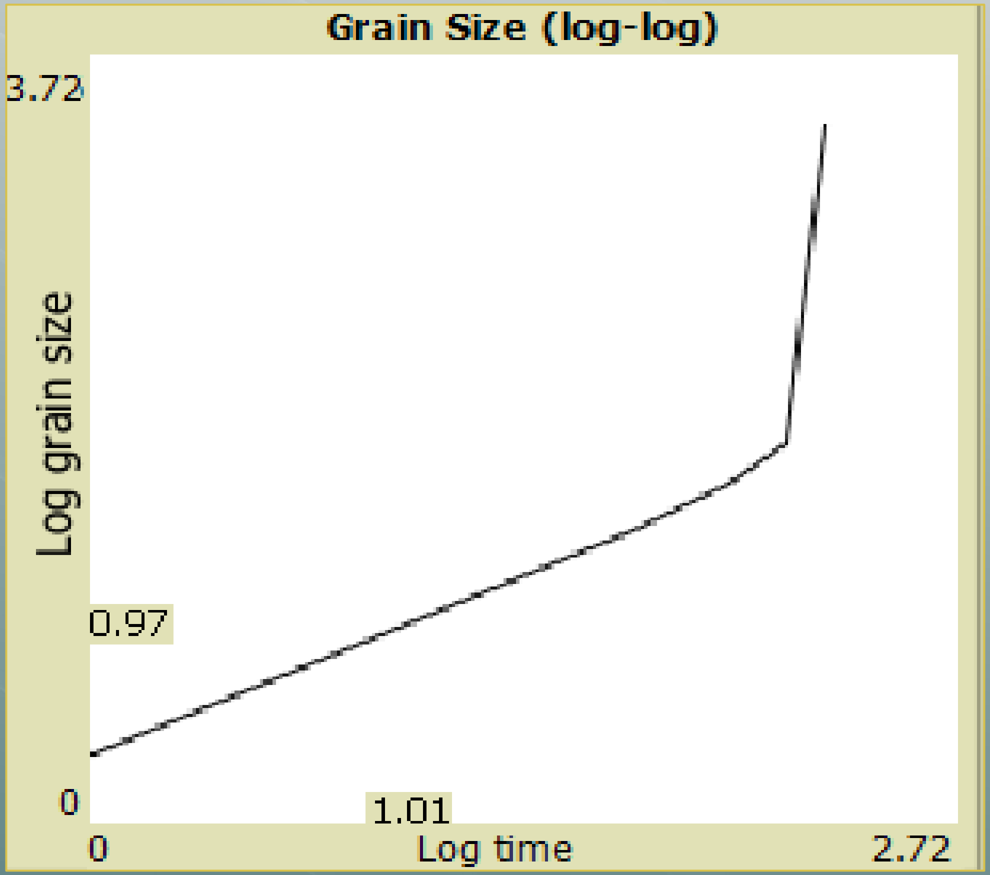
A Comparative Table of the Grain Growth of a Sapphire, Three Rubies, and a Diamond

T_{log_time}	T, s	N_s,mm	N_r, mm N_{rs}	N_{rm}	N_{rd}	$N_{d,}$ mm
0.5	3	5.2	4.6	5.5	5.5	4.5
1	10	9.5	8.0	10.0	10.0	9.5
1.5	32	16.2	13.8	19.1	15.5	20.0
2	100	32.4	17.8	40.0	34.7	38.0

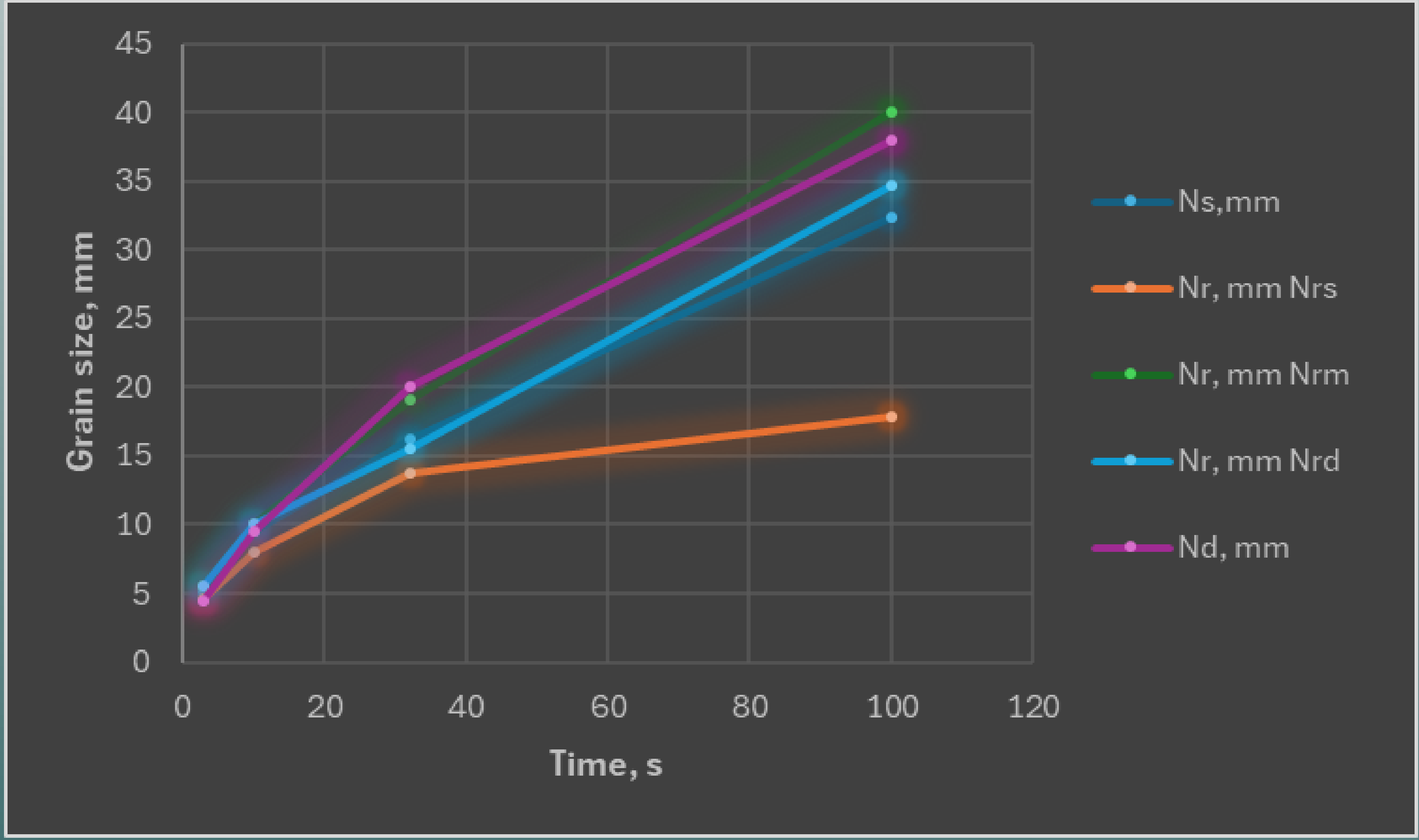
- **N_{rs}** – the grain size of a synthetic ruby;
- **N_{rm}** – the grain size of a nature ruby from Mozambique;
- **N_{rd}** – the grain size of the most precious ruby from the type “dove blood”;
- **N_d** – the grain size off a yellow diamond.

Graphics of the grain growth of sapphire and diamond generated in NetLogo 6.4.0 at T = 10 s.





A comparative grain growth diagram of all the sapphire, ruby, and diamond crystals.



IV. Conclusions and Scientific and Applied Contributions

- The comparison of sapphire and diamond crystals for laser applications can provide valuable insights into the behavior of these materials in various conditions.
- Simulating the growth of various crystals in terms of grain growth can offer important information for understanding the potential impact on laser performance.

Trends for Future Research

- Conducting extended experiments may contribute to the evaluation of how the faster grain growth of some gemstones affects the specific parameters and technical requirements of the laser systems, as it can have both positive and negative aspects depending on the objectives and the requirements.

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THANK YOU!

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