Rigid olivine fracture from the microscopic to the mesoscopic scale: Addressing the energy problem of earthquakes

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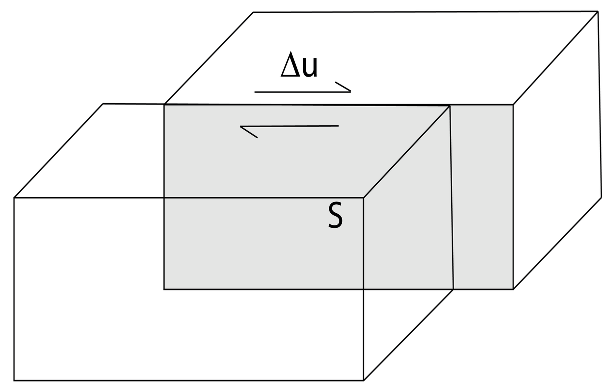
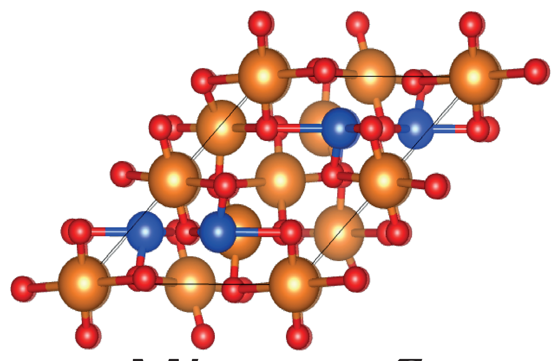
Accurately determining the total energy released by an earthquake represents a significant milestone that, unfortunately, has not yet been achieved. Seismology enables access to the component of energy radiated by an earthquake, but the values of other energy terms remain unknown. Being able to ascertain the total energy released during an earthquake has significant implications for the study of seismic risk, the development of early seismic warning systems, and consequently, damage prevention. Subduction zones are tectonic structures formed at the convergence of plate boundaries. The common mineral in subduction slabs is olivine, a magnesium ferrosilicate. The purpose of this work is to investigate the brittle rupture process of crystalline olivine from an atomistic perspective and estimate the energy involved in this process. This study is based on ab initio calculations following the Density Functional Theory (DFT) scheme. As a first step, the electrostructural energy minimum of the olivine's unit cell at 24 GPa (at a depth of 700 km) has been calculated. To obtain stress-strain curves, the relaxed unit cell has been subjected to shear distortions. Thus, it has been possible to calculate the theoretical total energy released during an atomistic-scale brittle rupture. To compare the atomistic energy budget with a macro-scale rupture mechanism (fault size), a fracture model at different scales has been developed. This has made it possible to simulate multiple grain ruptures, where each grain contains different crystallographic directions. The link between the micro and macro scale has been established by applying a stochastic simulation scheme for the multiple grain ruptures and estimating the energy released by an earthquake. The results have been compared with data from deep earthquakes in the Peruvian-Brazilian subduction zone.

1) From macroscopic to microscopic earthquakes

Have you ever wondered what is the difference between microscopic and macroscopic earthquakes? In this poster, we tried to answer this question by making hypotheses wich allowed to link together the microscopic and macroscopic ruptures.



$$M_0=\Delta u \mu S$$

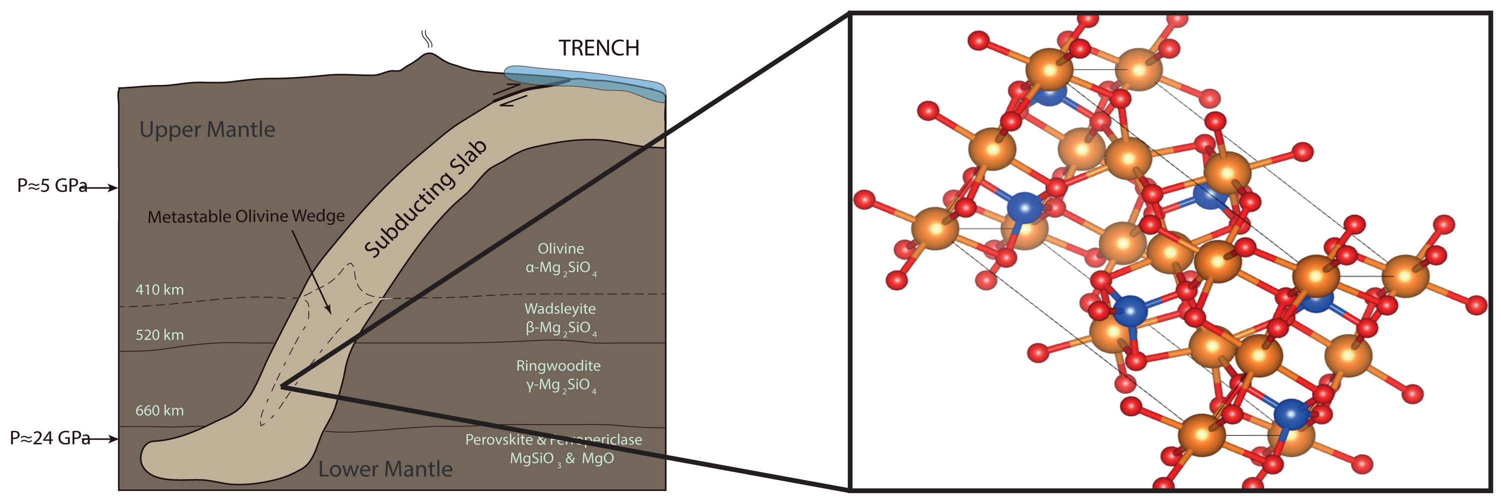


$$M'_0=\sigma_{ij}u_{ij}S$$

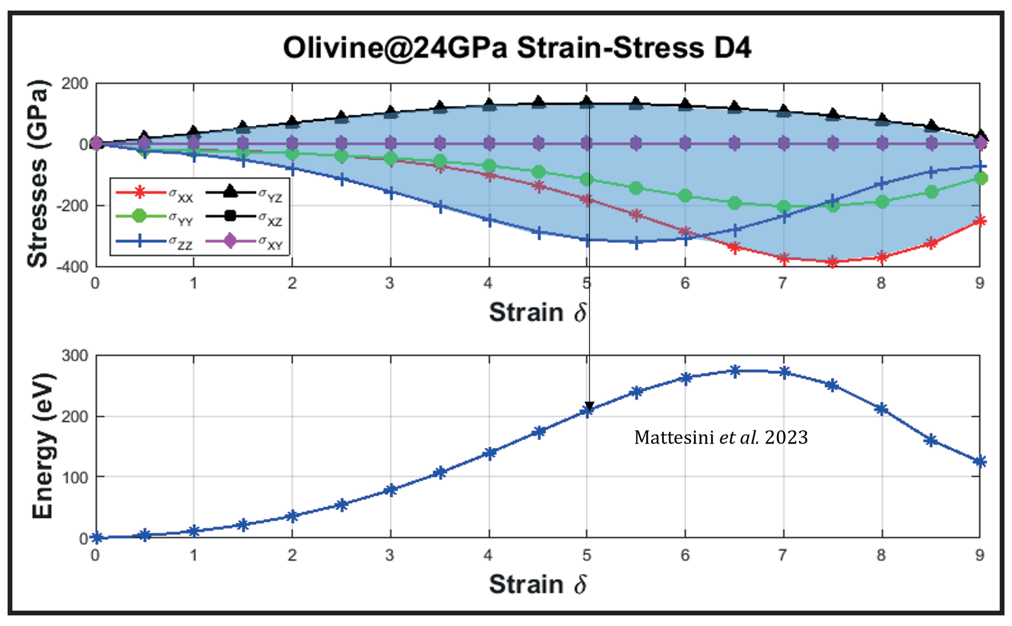
The left figure shows the macroscopic movement during a fault rupture. The right figure represents the atomistic deformation of an olivine unit cell.

2) Microscopic approach

Deep earthquakes are common in subduction zones. The initial hypothesis is that the seismogenic material in these areas is metastable olivine.



Subduction zone down to a depth of 660 km (Left). Olivine unit cell. (Right).



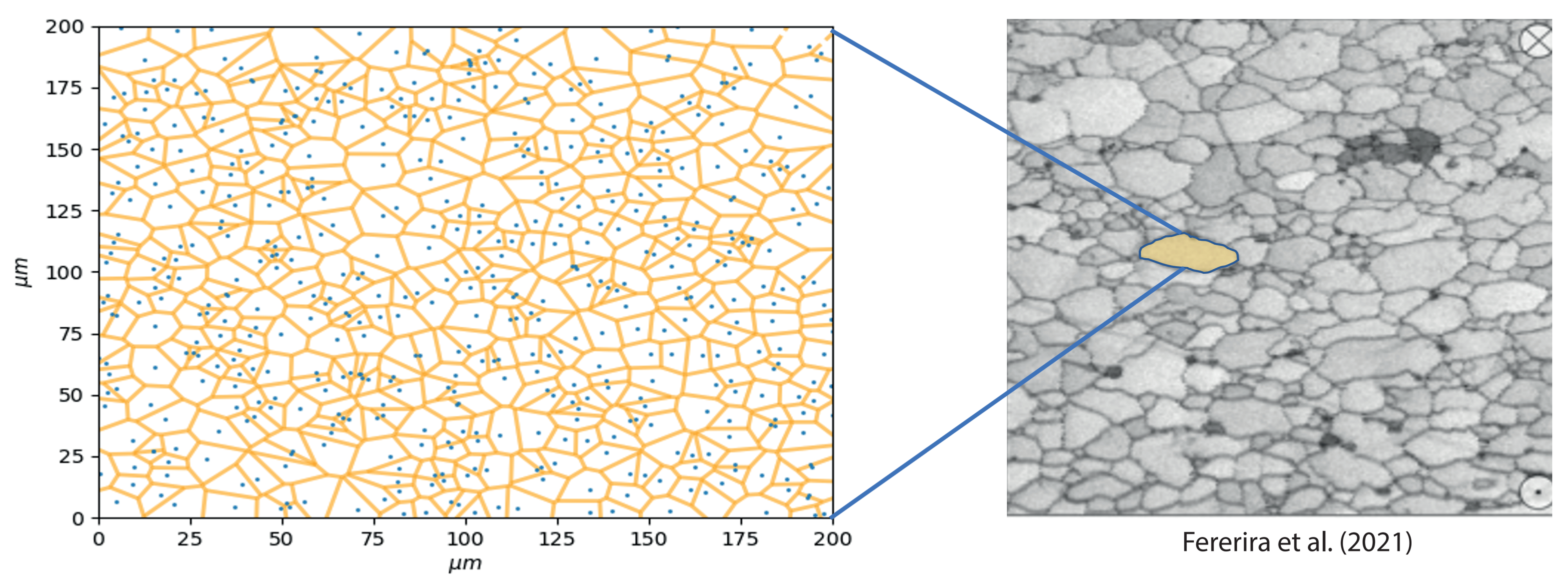
The upper panel shows the evolution of stresses vs. strain parameter (δ) for one of the volume conserving monoclinic strains. The lower panel represents the variation of the cell energy against the strain parameter.

Elastic constants @24GPa	
C_{11} (GPa)	294.56±4.93
C_{12} (GPa)	146.01±3.48
C_{13} (GPa)	139.92±3.48
C_{22} (GPa)	325.59±4.93
C_{23} (GPa)	143.43±3.48
C_{33} (GPa)	453.53±4.93
C_{44} (GPa)	105.96±3.98
C_{55} (GPa)	106.65±3.98
C_{66} (GPa)	103.98±3.98
B (GPa)	211.76
μ (GPa)	104.78
E (GPa)	269.84
V_s(km/s)	5.61
V_p(km/s)	10.28

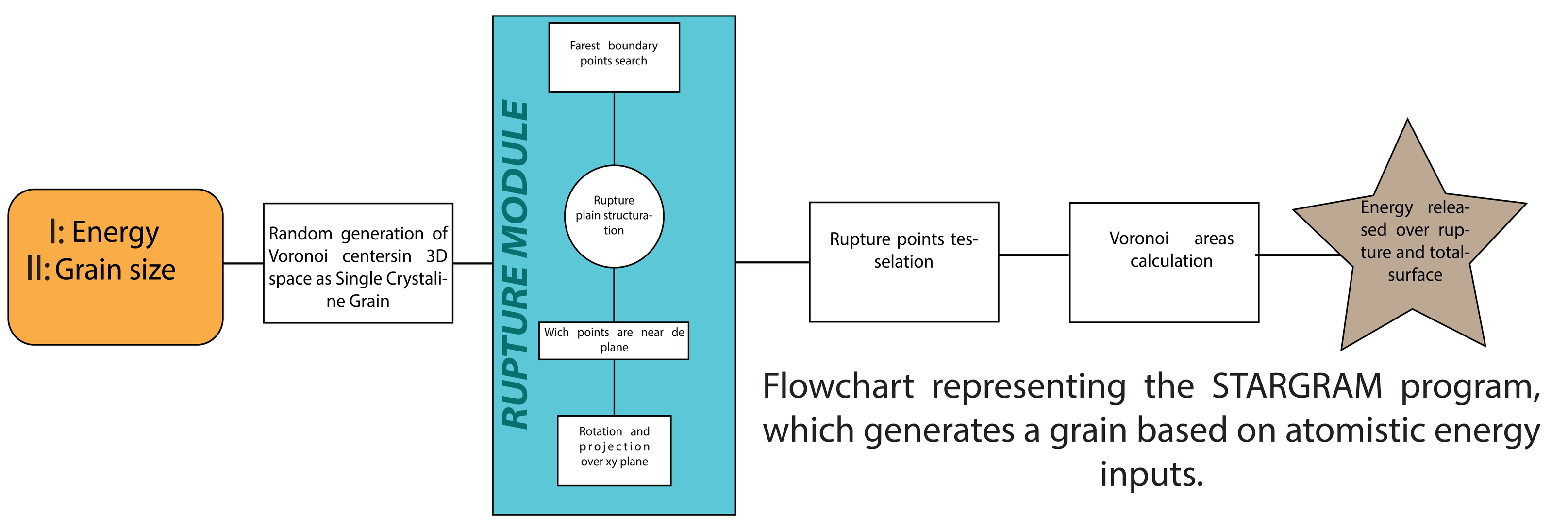
The table shows the elastic constants of olivine using quantum mechanics (DFT) from Mattesini *et al.* 2023.

3) Stochastic Atomistic Rupture in Granular Media: STARGRAM

We have simulated a crystalline grain using a stochastic approximation, taking the microscopic energy and grain size as inputs (Ferreira *et al.*, 2021).



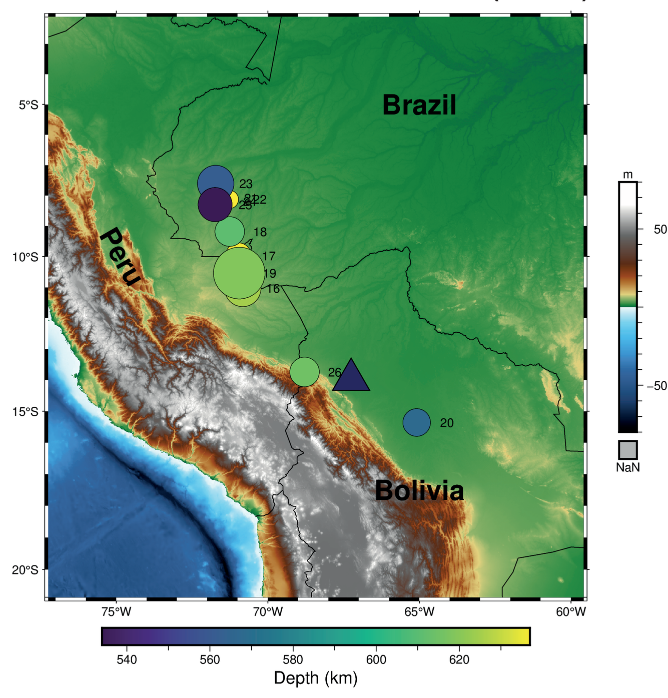
The righ figure corresponds to a TEM image (200 microns x 200 microns) of an olivine xenolith. The one on the left is a representation of the crystallographic energy domains generated through Voronoi tesselation.

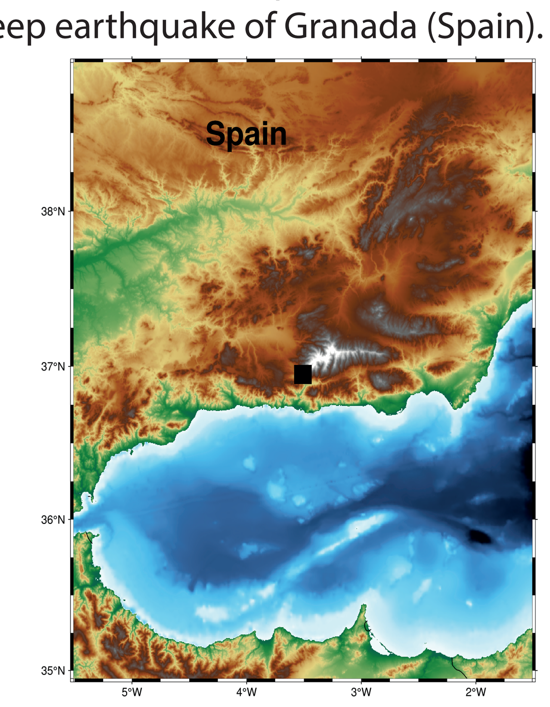


Flowchart representing the STARGRAM program, which generates a grain based on atomistic energy inputs.

4) Seismic data

The ultimate purpose of this work is to test STARGRAM into bridging microscopic atomistic fracture energies and macroscopic seismic observations. Therefore, this model will be compared with earthquakes in the Peru-Brasil border zone (PBBZ) and the 2010 deep earthquake of Granada (Spain).

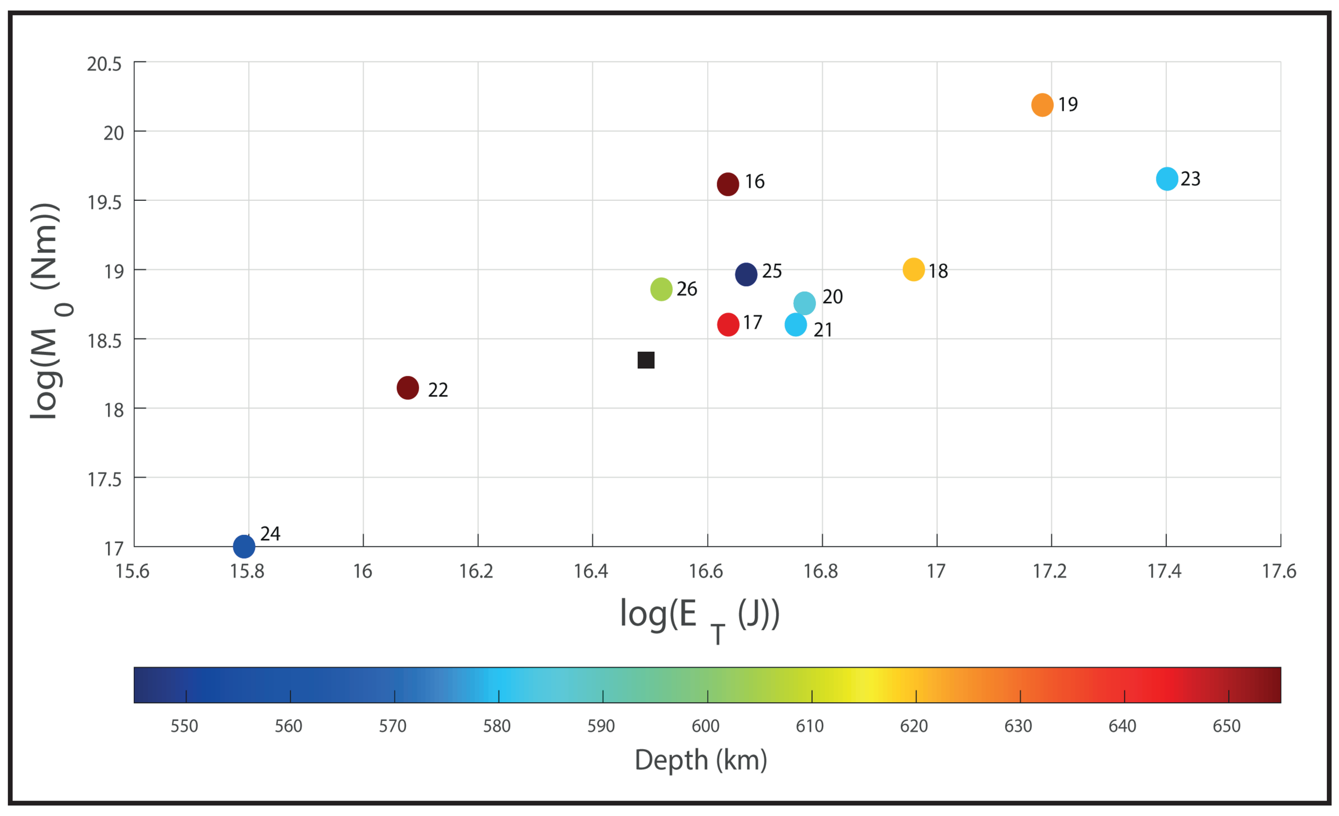




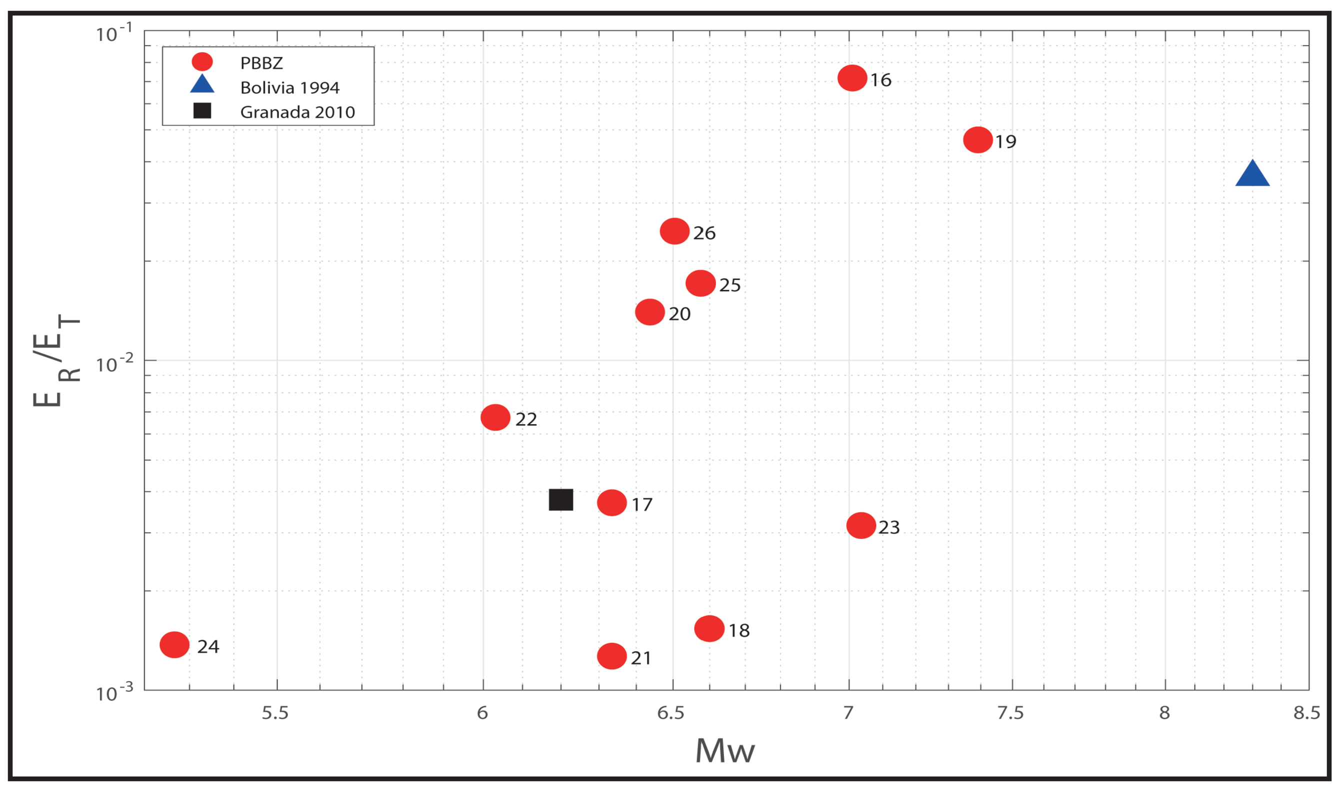
The size represents the magnitude of the earthquake, and the colour scale on the PBBZ earthquakes indicates the depth. The 2010 Granada earthquake occurred at a depth of 650 km with a moment magnitude of 6.2.

5) Dataset implementation and results

We have probed the STARGRAM program on the previously mentioned set of earthquakes.



Correlation between observed seismic moment and theoretical total energy.



Seismic efficiency $\eta = E_R/E_T$, calculated with the seismic radiated energy and the total theoretical energy in relation to the magnitude. Additionally, the earthquakes in Bolivia in 1994 (Kikuchi & Kanamori 1994) and the deep 2020 Granada earthquake (Buforn *et al.* 2011) have been included.

6) Conclusions

1) We have built an atomistic method that bridges microscopic fractures to macroscopic seismic observations (i.e., earthquakes)
2) We probed the new methodoloy for earthquakes in the PBBZ and for the 2010 Granada deep earthquake.
3) Results seem to indicate that Mo vs. E_T is almost linear and η folds within the range of 10^{-1}-10^{-3}.
4) Future developements will include glassy olivine layers at grain boundaries.

Buforn, E., Pro, C., Cesca, S., Udias, A., del Fresno, C., 2011. The 2010, Granada, Spain deep earthquake. Bulletin of the Seismological Society of America 101, 2418–2430.
Ferreira F, Hansen LN, Marquardt K. 2021. The effect of grain boundaries on plastic deformation of olivine. J. Geophys. Res. Solid Earth 126(7).
Kikuchi, M., and H. Kanamori (1994). The mechanism of the deep Bolivia earthquake of June 9, 1994, Geophys. Res. Lett. 21, 2341–2344.
Mattesini, M., Sánchez, C. L., Buforn, E., Udías, A., de la Serna Valdés, J., Tavera, H., & Pro, C. (2023). From an atomistic study of olivine under pressure to the understanding of the macroscopic energy release in earthquakes. Geosystems and Geoenvironment, 2(1), 100108.

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