



Ice Core Science Meets Computer Vision: Challenges and Perspectives

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Polar ice cores play a central role in studies of the earth's climate system through natural archives. A pressing issue is the analysis of the oldest, highly thinned ice core sections, where the identification of paleoclimate signals is particularly challenging. For this, state-of-the-art imaging by laser-ablation inductively-coupled plasma mass spectrometry (LA-ICP-MS) has the potential to be revolutionary due to its combination of micron-scale 2D chemical information with visual features. However, the quantitative study of record preservation in chemical images raises new questions that call for the expertise of the computer vision community. To illustrate this new inter-disciplinary frontier, we describe a selected set of key questions. One critical task is to assess the paleoclimate significance of single line profiles along the main core axis, which we show is a scale-dependent problem for which advanced image analysis methods are critical. Another important issue is the evaluation of post-depositional layer changes, for which the chemical images provide rich information. Accordingly, the time is ripe to begin an intensified exchange between the two scientific communities of computer vision and ice core science. The collaborative building of a new framework for investigating high-resolution chemical images with automated image analysis techniques will also benefit the already wide-spread application of laser-ablation inductively-coupled plasma mass spectrometry chemical imaging in the geosciences.

Keywords: ice core analysis, chemical imaging, laser ablation inductively-coupled plasma mass spectrometry, image analysis, scale spaces, co-localization, grain boundaries

1 INTRODUCTION

Ice cores drilled on the polar ice sheets are among the most important climate archives, delivering valuable insights into the complexity of our climate system (Fischer et al., 2021). With the deposition of snow, additional properties of the atmospheric composition (aerosols, stable water isotopes, etc.) are archived. When snow is transformed to ice, air bubbles are enclosed, providing actual snapshots of the atmosphere of the past and constituting a stand-alone feature of this natural archive. As a result, there exists a chemical and physical stratification of polar ice, which makes up the paleoclimatic record, which we shall refer to as “the stratigraphic layering”. The layering encoding this record is subject to changes with time and depth: the interaction between the paleoclimatic record and its preserving ice matrix extends from km-scale ice flow over millennia, down to the microscopic scale of interactions between impurities and ice crystals (Faria et al., 2010).

Glacier ice generally consists of a large number of individual crystals, or “grains”, as well as associated microscopic features such as grain boundaries and triple junctions, where three grain boundaries intersect. The microscopic localization of impurities with respect to the configuration of grains and their boundaries can crucially affect not only macroscopic deformational properties, but also the paleoclimate records: For instance, diffusion and segregation of soluble impurities into grain boundaries may alter or even destroy the sequence of paleoclimate signals (Rempel et al., 2001; Barnes and Wolff, 2004; Ng, 2021). Therefore, a quantitative study of the ice stratigraphy at the microscale, in particular the 2D distribution of chemical impurities, is crucial to understand how climate signals have been conserved or transformed, within the flowing ice over tens to hundreds of millennia. This is of particular relevance for the retrieval of novel climate records from the deepest, oldest and thinnest layers, the primary target of the upcoming ambitious “Oldest ice” ice core drillings in Antarctica, which is a grand challenge in the ice core sciences (Brook et al., 2006; Fischer et al., 2013).

Ice core stratigraphy can be assessed through a variety of methods. The most common approach is direct visual inspection, combined with microstructural analysis of selected ice sections *via* optical microscopy. Such datasets have revealed new insights into the complexity of the underlying physical processes, challenging established glaciological concepts (Kipfstuhl et al., 2009; Faria et al., 2014). Initial contact points with automated image analysis have now been developed. Early studies used coaxial reflected light and the birefringent properties of ice in visual images to automatically detect grain boundaries *via* image segmentation (Arnaud et al., 1998; Gay and Weiss, 1999). For datasets from directed bright-field illumination, a machine learning approach was developed to obtain automatic, reliable classification of ice crystal features (Binder et al., 2013). At the microscale, a digital form of optical microscopy was combined with automated image analysis to quantify the collective grain as well as bubble structure (Kipfstuhl et al., 2009; Ueltzhöffer et al., 2010; Bendel et al., 2013). Morcillo et al. (2020) recently employed digital image analysis for a macroscopic counterpart of dark-field microscopy to investigate the optical stratigraphy of an Antarctic ice core.

To fully assess the preservation of the climatic signals represented by the vertical distribution of impurity concentration in ice cores, jointly evaluating the chemical information with visual analysis is key. However, all techniques based on the chemical analysis of ice core meltwater lack the ability to directly assess lateral spatial relations among impurities within the ice, and face fundamental limitations in depth resolution (e.g., Breton et al., 2012). To analyze samples in the frozen ice state, scanning electron microscopy/energy dispersive X-ray spectrometry (e.g., Baker and Cullen, 2003; Barnes et al., 2003; Iizuka et al., 2009) as well as micro-Raman spectroscopy (e.g., Eichler et al., 2019) have been successfully used to determine the location of impurities within the ice matrix and to analyze the chemical composition of individual particles, typically based on spot-like measurements. The evaluation of the chemical micro-

stratigraphy and its implications for the interpretation of coarser scale meltwater signals requires continuous 2D information. However, a standard technique in 2D chemical imaging has not yet been established for ice cores.

A highly promising candidate in this regard is LA-ICP-MS. LA-ICP-MS uses a laser to ablate a few tenths of micro-liters of ice from the surface, which are subsequently analyzed for various elemental impurity species with a mass spectrometer (Müller et al., 2011; Sneed et al., 2015; Della Lunga et al., 2017; Spaulding et al., 2017). Very recently, the application of LA-ICP-MS for 2D chemical imaging in ice cores has been refined and greatly improved (Bohleber et al., 2020a). Here high-resolution artifact-free 2D images from state-of-the-art imaging methods (e.g., Wang et al., 2013; van Elteren et al., 2019) provide an unprecedented density of information; several million laser shots (correlating with chemical measurements) are fired over just a few square mm. A camera co-aligned with the laser then captures visual images of the ice sample surface. By this means, LA-ICP-MS combines chemical and visual information of the ice core microstratigraphy.

The introduction of a new technology establishes the need for better understanding the potential and limitations of these novel high-resolution 2D chemical images of ice cores. As we see new frontiers of multidisciplinary research emerging in this framework, the employment of computer vision methods might be a game-changer for fully exploiting the complexity of the chemical images. In the same fashion as computer vision has lead to advances in medical image analysis, neuroscience, biomedicine, robotics, object recognition, and a host of other areas, the time is ripe for it to revolutionize ice core science. To accelerate this, in this article we begin an inter-disciplinary dialogue. We describe a selected set of key problems in the analysis of chemical images of ice cores as examples of future inter-disciplinary research questions, that can only be successfully tackled in close collaboration with the computer vision community.

2 MAKING CHEMICAL IMAGES OF ICE CORES

Impurity images are acquired as a pattern of lines, without overlap in the direction perpendicular to that of the scan, and without any further spatial interpolation. Each pixel in an ice core chemical image has a size of $35\ \mu\text{m} \times 35\ \mu\text{m}$ (Figure 1). For each chemical element a numerical matrix contains rows and columns, according to the physical size of the image: an image of $7\ \text{mm} \times 35\ \text{mm}$ in size has 200 rows and 1,000 columns. The numerical entries in this matrix refer to either the recorded intensity (e.g., counts per second) or, if a calibration is applied, the concentration (e.g., in parts per million). Due to the careful synchronization, the individual pixels of the different chemical channels can be considered to be almost perfectly spatially aligned. In contrast, the mosaic of visual images obtained from the laser camera is not a-priori aligned with the chemical images. A sample dataset (including the datasets from Figure 1) has been made publicly available (see data availability below). Details on

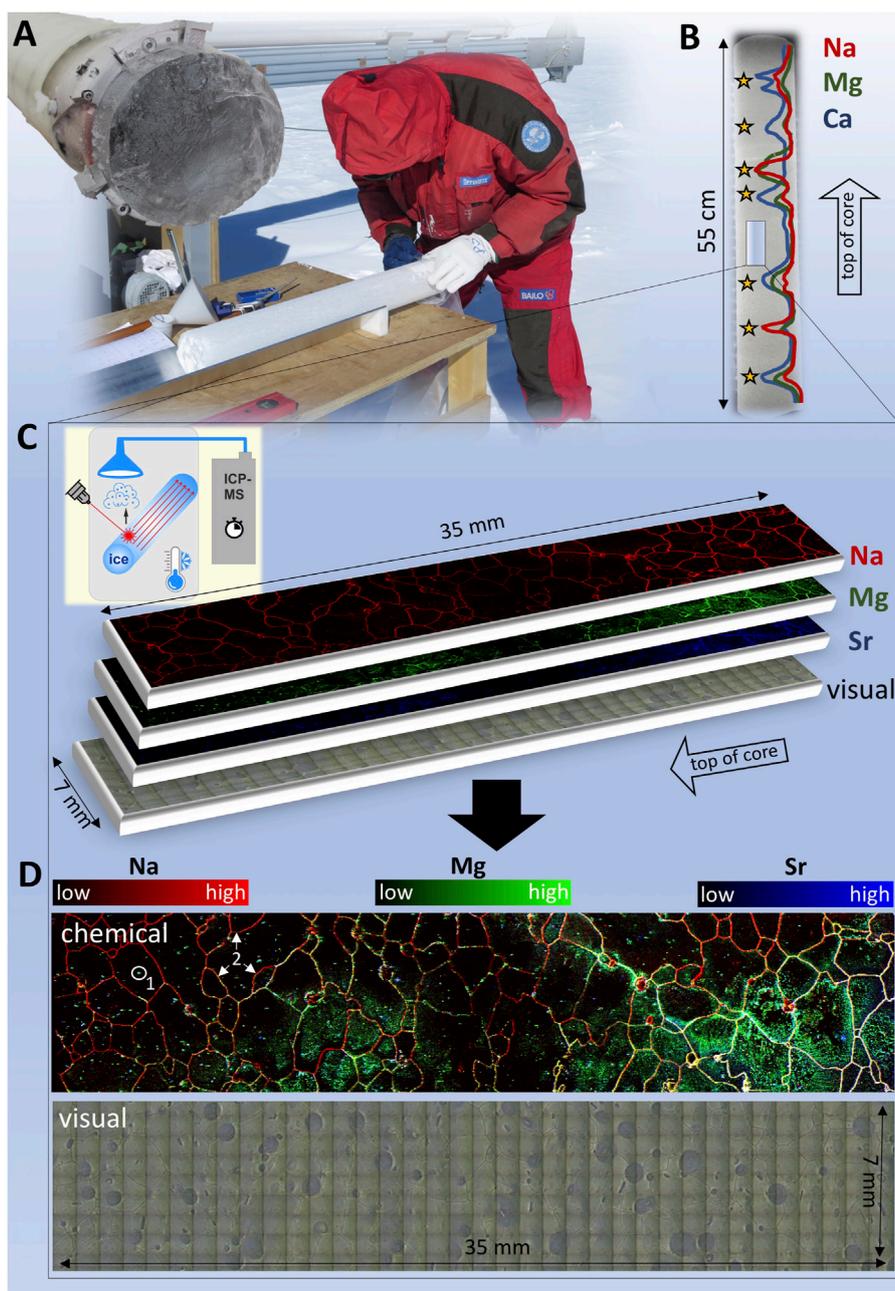


FIGURE 1 | Laser-ablation inductively-coupled plasma mass spectrometry imaging at micron-scale resolution combines new chemical dimensions with visual ice core analysis. Shown in **(A)** is an ice core drill and a freshly drilled ice core piece. Typical cm-resolution signals of chemical impurities obtained from meltwater analysis are illustrated in **(B)** (photo credit: Sarah Wauthy). Stars (★) indicate hypothetical stratigraphic (e.g., annual) layers. Row **(C)** shows the chemical imaging with LA-ICP-MS, with examples for the chemical image for Na, Mg, and Sr intensities, using separate color channels and the visual images obtained from a mosaic of camera images [in **(D)**]. The comparison shows individual bright spots 1) and that the network of lines most dominant in the red Na image 2) correspond to the grain boundaries which are seen as dark lines in the visual image. Background image in tile A: copyright PNRA.

the imaging technique are described elsewhere (Bohleber et al., 2020a).

The visual images are generally characterized by air bubbles (dark blobs), grain boundaries (dark lines), and occasional sub-grain boundaries (thin dark lines). In the chemical images, the individual impurity channels generally differ, e.g., through a

variable degree of impurity localization at grain boundaries, depending on the depth sections and respective climatic period. The LA-ICP-MS image shown in **Figure 1** has been obtained from the EPICA Dome C deep Antarctic ice core, on a sample from a glacial period of about 27.8 thousand years ago. Additional images are presented elsewhere (Bohleber et al.,

2020b). From a conceptual point of view, **Figure 1** is a representative example of the following general image characteristics: i) Small bright spots of a few ten microns occurring within grains as single spots or in small clusters. “Clouds” of such spots are also observed. ii) High intensities reflected in co-localization with the grain boundary network, especially for the Na images. In a typical 7 mm × 35 mm image, tens of grains to a few hundred grains can be distinguished visually. iii) Overall intensity gradients on the mm-scale, showing sections with darker versus brighter intensities.

3 KEY QUESTIONS AND A ROLE FOR COMPUTER VISION

The future technological evolution of LA-ICP-MS ice core analysis promises to increase image size by at least one order of magnitude or more, enabled by large cryocells (Sneed et al., 2015) and faster scan speeds (Šala et al., 2020). With more chemical channels added, the results are high dimensional images that call for an equal advance in data reduction and interpretation. This way, the chemical images may provide important new insight into the identification and preservation of paleoclimate signals in deep ice, one of the pressing challenges in today’s ice core research. Below we discuss three crucial questions that connect the analysis of the chemical images to this challenge, illustrating where the application of computer vision methods could lead to breakthroughs.

3.1 Question 1: Can Scale-Space Theory Assist in Extracting Paleoclimatic Signals?

Previous investigations focused on establishing a meaningful interpretation of the novel LA-ICP-MS signals through a validation against existing meltwater analysis. It was shown that the coarse-scale variability seen in 1D single line profiles of LA-ICP-MS, measured along the main core axis, is consistent with the full resolution signals from meltwater analysis (Della Lunga et al., 2017; Spaulding et al., 2017). The coarse-scale variability had to be inferred by applying substantial (e.g., Gaussian) smoothing to 1D single line profiles. In this fashion annual layers could be identified (i.e., the chemical contrast between summer and winter snow layers) which were thinned beyond the cm-resolution capabilities of meltwater analysis (Bohleber et al., 2018). However, smoothing with a Gaussian simply discards much of the high-resolution signal, and crucial information is potentially lost.

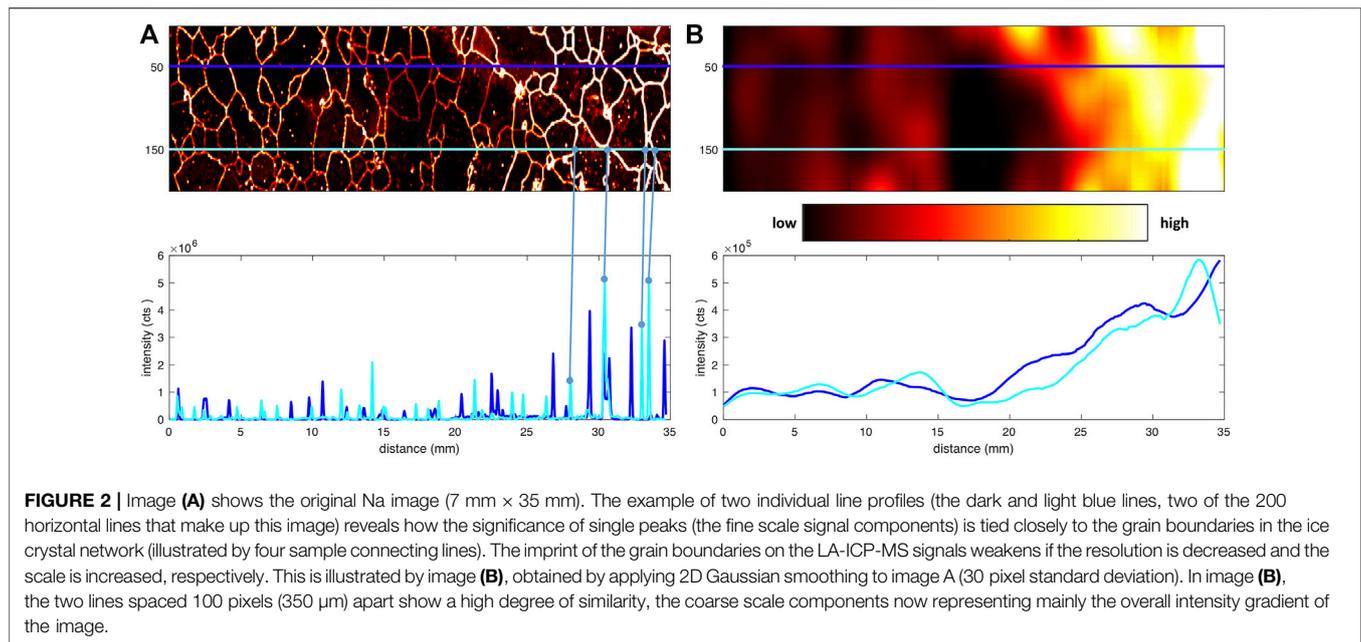
Initial evidence has already suggested a relationship between the fine-scale signal components (e.g., peaks in 1D line profiles) and the grain boundaries (Della Lunga et al., 2014; Kerch et al., 2015; Beers et al., 2020). The new 2D imaging technique has fully revealed the influence of ice crystal features and has demonstrated that, if an impurity species is mostly localized at the grain boundaries (such as Na), it is in turn the grain boundary network that determines the fine-scale signal components in single line profiles (Bohleber et al., 2020a).

Accordingly, there should exist a hypothetical “sweet spot” in measurement scale, at which the stratigraphic record (e.g., annual layers) is captured at the highest possible resolution, while the imprint of crystal-related features such as grain boundaries is still avoided.

However, the physical scales of stratigraphic layering and ice crystal features are neither constant in depth nor universal among all cores: the stratigraphic layering becomes increasingly compressed with age and thinned due to deformation by ice flow. The size of ice grains also varies between glacial and interglacial periods, and can become increasingly large in deep ice due to several processes. Eventually sub-mm (annual) layer thickness can be expected in ice, showing grain diameters exceeding several cm (Faria et al., 2010; Fischer et al., 2013). This means that the localization of impurities at grain boundaries can ultimately erase the original layer sequence. In this case the crystal size becomes an upper limit to the resolution at which the related paleoclimate signals may be interpreted. Accordingly, to separate the imprint of ice crystal features from the stratigraphic layering may not be achievable in all instances, especially once the stratigraphic signal gets corrupted by layer folding, impurity segregation to grain boundaries and migration along the ice vein network.

As a starting point to tackle this question, undisturbed ice core sections typically feature a nearly level layer sequence (Svensson et al., 2005). In this case, signals related to the stratigraphic layering should not be a primary function of the lateral position of the line profile on the ice core surface (Sneed et al., 2015; Della Lunga et al., 2017). However, due to the presence of the grain boundary imprint, this does not hold at the high resolution scale, as shown in **Figure 2**. On the other hand, for the example of the Na image of **Figure 1**, the grain boundary imprint becomes increasingly blurred until, at a scale of around 1 mm (e.g., the standard deviation of the Gaussian kernel), only the overall intensity gradients of the image remain present. This suggests that the overall intensity gradient is connected to the stratigraphic layering, warranting further investigation. Small-scale folding would corrupt the above criterion, with regard to the lateral signal coherence. An answer cannot come from 1D line profiles alone, but rather requires an analysis of the 2D images.

Evidently, this question has a deep connection to the scale of the image features. Hence, much may be gained from treating this question with scale-space techniques, a well-established field in computer vision (Witkin, 1983; Koenderink, 1984; Lindberg, 1994; Florack et al., 1994; Florack et al., 1996; ter Haar Romeny, 2003; Duits et al., 2004; Koenderink, 2021) for which modern approaches leveraging deep learning are now emerging (Bekkers et al., 2018; Romero et al., 2020). The expected output from scale-dependent image characterization should allow one to optimize the experimental design to reliably detect the stratigraphic layer signal at the highest possible resolution. This can mean determining the physical resolution of analysis, such as the laser spot size, and determining the number of and lateral spacing between the parallel lines needed—ideally including a criterion for the detection of small-scale folding.



3.2 Question 2: What do Image Features Reveal About the Ice Core Record?

Detecting, counting and classifying grain boundaries, triple junctions and spot-type image features along the chemical image dimensions can offer new and improved ways of extracting chemical information. For instance, marine and terrestrial sources of insoluble particles have been distinguished based on a classification according to the multi-elemental composition (Oyabu et al., 2020). For the chemical images such a classification is a complex task that needs to be performed automatically, or it will be intractable with growing image size. Thus, this is another area where expertise from computer vision will be instrumental in overcoming the present limitations.

The chemical images also offer new options for the investigation of post-depositional chemical reactions. As a concrete example in this regard, meltwater analysis of a deep Antarctic ice core revealed that sharp sulfate spikes showed an “anomalous” chemical composition, which was explained by the post-depositional formation of soluble particles of magnesium sulfate salts in grain boundaries (Traversi et al., 2009). The latter process would imply the co-localization of Mg and Ca in grain boundaries. Chemical images can provide new insights about whether the *co-occurrence* of impurities in meltwater analysis is in fact a result of their *co-localization* at grain boundaries.

Since the chemical images will, for the foreseeable future, only cover a small representative section of a typical sample melted for analysis [e.g., approximately 1 m long, cross-section typically 3 cm × 3 cm (Röthlisberger et al., 2000)] a meaningful way of extrapolation and upscaling is needed when attempting a direct comparison to meltwater techniques. In this context, macroscopic variables derived from the images can be compared more easily to those of other datasets. Examples of

such variables are grain size and shape as well as the spatial density and chemical signature of insoluble particles (related to spot-type features). This can be compared, e.g., to visual datasets, volume particle concentration derived from macroscopic meltwater analysis and other chemical measurements.

Using image features (Zhou et al., 2016) in concert with tools including co-localization analysis, image segmentation (Kass et al., 1988; Malladi et al., 1995; Chan and Vese, 2001; Long et al., 2015; Ronneberger et al., 2015) clustering (Shi and Malik, 2000; Ng et al., 2002; Pavan and Pelillo, 2007) and object detection (Ren et al., 2015) can provide a foundation for performing such analysis in a quantitative manner. For instance, to assess the layer integrity, an algorithm must determine i) the degree of localization of an impurity species at the grain boundaries and weigh ii) the average size of the grains against iii) the thickness of the stratigraphic layering of interest. The latter data (expected nominal thickness of annual layers etc.) can typically come from existing datasets from glaciological and ice core analyses.

3.3 Question 3: Can Computer Vision Help to Test Existing Theories of Impurity Diffusion?

Impurities can diffuse especially along ice veins (i.e., the network of triple junctions) due to concentration gradients of soluble species or chemical competition (Barnes and Wolff, 2004). There is also the case of “anomalous diffusion” which can lead to 1D signal displacement along the main core axis (Rempel et al., 2001). Recently it has been shown that diffusive impurity transport along ice veins will lead to an effect much like low-pass filtering on 1-D signals (Ng, 2021). Hence, the diffusive impurity relocation is another crucial question, for which the chemical images may provide important detail if combined with computer vision techniques.

Evidently, whether the diffusive impurity becomes strong enough to affect the paleoclimate signals depends on two factors: i) the relative degree of localization at triple junctions (i.e., most of the impurities need to be located there) and ii) the connectedness of the ice vein network (vs. blockages or void areas). Regarding i), the position of triple junctions in the images can be determined either from visual data or from chemical images with a high degree of localization at grain boundaries, like Na. Various algorithms exist for triple junction detection. For the corresponding position of triple junctions, the relative intensity or concentration level can be determined and compared to levels at grain boundaries and grain interiors.

Regarding ii), the degree of connectedness of the ice vein network could be evaluated using a 3D approach. For this purpose, 2D images are stacked together, either in consecutive ablation or after removing a surface layer manually by scraping/polishing the surface (Van Malderen et al., 2017). This means that building a 3D model of the ice vein network may require some interpolation or statistical treatment of all detected triple junctions.

4 OUTLOOK

In future applications, fully automatic methods based on computer vision techniques may offer the speed and accuracy to systematically analyze the large-scale, high-dimensional datasets that modern acquisition systems will provide in the coming years. Once tools for investigating the key questions related to the chemical images have been developed, the ice core community could independently focus on their application, similar to the now established techniques for processing visual ice core images. Regarding a vision for a prolonged long term partnership between ice core and computer science, it can be envisaged that, once initial algorithms have been developed, a next step could involve further automation, e.g., to train a machine learning algorithm to recognize instances of stratigraphic layer disturbances in the chemical images. This would result in machine-based assistance similar to that in present state-of-the-art medical diagnostics. As the technology continues to evolve, large sized (square tens of cms) with tens of chemical dimensions may become a standard practice over the coming years. At that point, imaging of new ice cores could have produced thousands of images like the one shown in **Figure 1**, including dedicated platforms for data and code exchange. As thousands or millions of annotated or labeled examples become available (typically for classification or labeling tasks) deeper and wider neural networks can be used, as is now common for many modern day computer vision applications. Transfer learning, active learning, or domain adaptation techniques might help in lowering the labeling effort. However, we are presently quite

far from having such annotated data, or abundance of examples. This motivates the use of more classical computer vision and pattern analysis methods, as a starting point. Object detection could help in quantitatively analyzing the number and chemical characteristics of impurities at grain boundaries, triple junctions and other locations. Here, tasks such as interactive image segmentation or semantic segmentation could help automatically detect grains and their boundaries. Ultimately, computer vision has the potential to lead to a permanent transformation in the manner that chemical stratigraphy in polar ice cores is investigated. With the dialogue started here, we envision the formation of a new community spanning present disciplinary boundaries across geosciences, one which includes imaging and image analysis experts alike.

DATA AVAILABILITY STATEMENT

The data presented in the study are deposited in the Zenodo repository, <https://doi.org/10.5281/zenodo.4912280>.

AUTHOR CONTRIBUTIONS

All authors contributed to the discussion and the writing of the manuscript. PB, MR, and CB established the ice core chemical imaging. MP conceived the original idea behind this manuscript.

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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