Data Repository

Methods

<u>*Fieldwork*</u>

Soil Cores and other samples

In total, 96 micro-cores of Cryptogamic Ground Cover (CGC) soils and colonizing vegetation were collected from over 20 localities across Iceland. Here we present results from the three most contrasting sites. Micro-soils were cored using a cork borer (25mm x 80mm), and transferred to plastic vials, treated with 10% formalin, sealed, and are now stored at the Natural History Museum (NHM), London. Care was taken to avoid areas of extensive vascular plant growth which could potentially prove to be a source of 'contamination'. A representative sample of CGC plant species and lichens were also collected for identification purposes. Bryophytes found at each site are listed in Table DR1. Further details of the general bryology of Iceland can be found in Jóhannsson (1983) and Wilberscheid (2008).

Field localities

Sampling sites were chosen on the basis of substrate type, age of site, habitat, and community composition for a comparable sampling strategy of bryophytes colonizing a variety of substrates and habitats (Fig. DR1A; Arnalds, 2015). Soil mineralogical components were generally angular, with a size variation between 12mm and 36μm. Sampling at the Krafla Fires site (L1; Fig. DR1 B-D) occurred on numerous patches of moss and liverwort dominated loose substrate. Mosses tended to colonize the open areas, whereas liverworts colonized the shaded, damp areas. The substrate at the Krafla Fires site is better sorted compared with others, and comprises semi-rounded, vesicular and porous basaltic scoria clasts. At the Sólheimajökull moraine (L2) we sampled two surfaces at ca. 210° bearing from the retreating glacier snout (Fig. DR1E, F). These were chosen to compare the influence of different organisms colonising the moraine. Examination of aerial photographs from Google Earth and recent proximal volcanic eruptions (Eyjafjallajökull in 2010) indicate that the substrate was deposited within the last decade, although it is difficult to constrain an exact age. Substrates and soils at Sólheimajökull glacier are proximal to source and have undergone limited abrasion, and consequently they are poorly sorted and angular. The matrix is typically of clay-silt grade clast size. Sampling at the Snæfellsnes braided fluvial sequence (L3) occurred on exposed and bare mid-channel bars and densely colonized moss carpets (Fig. DR1 I-J) on the alluvial plain. The channel (~8m) was at a seasonally low level. Soils beneath CGC covers were <10 cm thick, unconsolidated and well-drained. We chose CGCs inhabiting loose substrates to obtain information on the very earliest stage of colonization and this effect on weathering.

CGCs composed predominantly of moss (e.g., *Racomitrium sp.*) can easily exceed 8cm in thickness, so we restricted sampling to thinner covers that were in contact with the soil surface. The nature of the CGC soil structure varied with plant growth form and the maturity of the site. The two principal exemplars of this were the liverwort dominated Sólheimajökull Glacier moraine CGCs (Fig. 1, L2) and the moss dominated Snæfellsnes Peninsula alluvial plain CGCs (Fig. 1, L3).

Identification of biologically-mediated weathering features

Iceland was chosen as a suitable field site because of its richness in easily weatherable detritus and the basaltic glass proportions in its soils (Arnalds, 2015). Because of it's generally 'unstable' chemical composition, basaltic glass exemplifies chemical and biologically-mediated alteration features readily. Glass grains were sought for two reasons: a) to homogenize the initial chemistry by looking at the same grain type, and b) because glass is naturally unstable and prone to rapid weathering.

One of the main methods of differentiating between biologically-mediated alteration and abiotic chemical weathering is that during chemical weathering, minerals preferentially dissolve along specific crystalographically determined planes (e.g., cleavage, denticulated margins; Hellend et al., 1997) having a predefined shape and orientation which is the result of the original chemical structure of the mineral (Landerweert et al., 2001). Biologically mediated features, however, are focused to a specific area, regardless of chemistry, although the chemically-determined structure of the grain/mineral could influence the route in which the bio-feature develops. In addition to this, all of our biologically-mediated structures have rounded/curved edges (e.g., Hoffland et al., 2004), which is potentially a primary indicative feature. Biological weathering features can also take on or reflect aspects of the morphology of the organism. Thus, bifurcating parallel sided tunnels within mineral grains or trenches on the surface of grains reflect the growth of fungal hyphae (Fig. 3D). We therefore interpret the 'bowls', 'grooves' and non-symmetrical holes as surficial biologically-mediated weathering features, and the penetrating 'borings' and 'tunnels' as internal biologically-mediated features. Thus the primitive chemical composition of the detritus in Iceland, together with the 'recent' formation times, provides an excellent 'natural laboratory' to study early colonization and weathering processes.

SEM imaging

Scanning Electron Microscope (SEM) imaging was conducted on two different SEM machines; a Leo 1455 Variable Pressure SEM and the high resolution FEI Quanta 650 FED SEM within the Core Research Laboratories at the NHM, London. Two SEMs were used because of the higher quality imaging of raw samples under variable pressure on the Leo, and higher quality imaging of coated samples under high vacuum on the Quanta. Whole mineral/glass grains, plants, and thin sections were all imaged under the SEM, some grains also having corresponding micro-organisms (cyanobacteria, fungi, algae, diatoms) still attached. Thin sections provided a 2D view of structures as opposed to grains in 3D. Samples were air dried and mounted onto sticky carbon pads on SEM stubs. In total, over 200 images were collected from 27 samples, however only a small number of images exhibiting the discussed biologically-mediated features are presented in this paper. Grain markings and features were sought that were associated with biotic material (particularly rhizoids) and micro-organisms. Variable pressure mode was preferred to avoid shrinking of any biological material that may have been present on the grains. Some samples were sputter coated with gold/palladium on a Cressington 208HR sputter coater to a layer 15 nm thick across the surface of the grain to enable imaging to a better resolution (up to 200nm or ~70,000x magnification) on the Quanta compared with using variable pressure on both the Quanta and the Leo (up to 3μm or 6,000x magnification). Thin sections remained uncoated for continued separate study by light microscopy. Average image values for the following parameters are listed here: kv (10 kv), working distance (15 mm), low pressure (Quanta: 60 Pa, Leo: 20 Pa), high pressure (Quanta: 1.21e-3 Pa), spot size (Quanta: 3 μm, Leo: 550 nm). Details of these parameters for each image discussed in the main text are illustrated in Table DR2.

SEM EDX analysis

Geochemistry was determined from scanning electron microscope energy dispersive X-ray (SEM-EDX) analysis. Analyses were performed on both the Leo and the Quanta SEMs under backscattered electron (BSE) mode. The Leo is equipped with a four-quadrant solid state backscattered detector, a variable pressure secondary electron detector, and an energy dispersive X-ray (EDX) detector (Oxford Instruments X-Max detector). The Quanta is equipped with a Bruker Flat Quad 5060F energy dispersive x-ray detector. Both raw grains and thin sections where analysed, however the coated samples were not. Analysis was undertaken on unprocessed grains. Clean areas are those that are judged to be free from physical indicators of alteration, etching, and secondary mineral development.

Analyses were undertaken in spot mode for point and line analysis. 30 spot analyses were performed on each analysed area to obtain average compositions. Analyses were obtained at an average magnification of 10,200x, and each individual spot measurement had a spot size of 50nm. Other average parameters include: 10kV, a probe current of 0.5nA, 100 seconds live time per spot analysis, and an average count of 18,630 per spot. Geochemistry of major elements was totalled to 100% by a stoichiometry method. Resulting analyses were reconstructed using Oxford Instruments INCA software.

In our analysis of biologically-mediated weathering features we needed to reference the background primary composition of the mineral grain. To do this, we identified and took additional comparative measurements from freshly fractured and clean areas of the glass grains. These are areas which, from inspection, had not undergone significant abiotic or biotic weathering were taken to represent the initial chemistry of the glass. The small standard deviation between the analysis and averaging of 30 spot analyses at each site suggests that the use of this data was justified and that it represents as close to the initial chemistry of that particular glass grain as was physically possible.

X-ray micro-CT (µCT)

μCT was used to reveal CGC soil structure and the relationship of colonizing organics to substrate. In total, 31 micro-cores were scanned on a Nikon Metrology HMX ST 225 micro-CT scanner using a tungsten reflection target and a 0.5mm copper filter at 140kV, 500ms exposure and 140μA. 3142 projections were collected, and a scan time of ~35 minutes. The average voxel size was 23μm, the lowest being 5μm. Scans were reconstructed using CT Pro Software (Nikon met., Tring) and rendered in VG Studio Max v2.1 (Fig. 2A-C) and Drishti v1.9 (Fig. 2D). 3D reconstructions were rendered for study, as well as 2D slices through each projection. All scanning was performed within the Core Research Laboratories at the NHM, London. The advantage of using μCT is that it's non-invasive, and it provides an image in three dimensions of the spatial arrangement of key elements of the soil (e.g., larger organics, clasts). It also enabled us to precisely identify the spatial relationship between particular plants and clasts, enabling chemical analysis of clasts of known orientation and proximity to known organic structures (e.g., rhizoids).

XRD

Clay mineralogy was measured on a Panalytical Scanning Diffractometer X'Pert Pro MPD Alpha1 X-ray diffractometer (XRD). It is equipped with a primary monochromator and para-focussing optics for high resolution measurements using Cu radiation. Samples were first powdered and mounted as oriented mounts for general analysis. Samples were then glycolated and mounted on glass slides. Sample preparation for this consisted of extracting the clay-sized fraction (<2μm) via a centrifuge and mounting the resulting fraction onto a glass slide. Samples were left to dry and then housed in a glycolating desiccator in an oven at 80°C for 24 hours prior to analysis.

References

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Figure captions

Figure DR1: Images of field localities. A-C: Site L1 (Krafla Fires), D-G: Site L2 (Sólheimajökull Glacier), H-I: Site L3 (Snæfellsnes Peninsula). A: Extensive moss carpet in Krafla Fires lava field. B: Example of moss-colonized areas on loose volcanic substrate. C: Small patches of thallose liverworts inhabiting loose volcanic substrate. D-E: Google Earth images of sampled locations at Sólheimajökull glacier; Red square in D highlights zoomed area of E. F: Thallose liverwort (*Blasia pusilla*) colonizing loose moraine at sampling site 1. G: Better developed moss carpets at sampling site 2. H: Sampling site at Snæfellsnes Peninsula. Mid-channel bar (black arrow) and moss carpet (white arrow) illustrated. I: Moss carpet cross section illustrating CGC soil structure.

Figure DR1 - Field images from: sites L1 (N. Krafla Fires; A), L2 (Sólheimajökull glacier; B), and L3 (Snæfellsnes Peninsula; C)

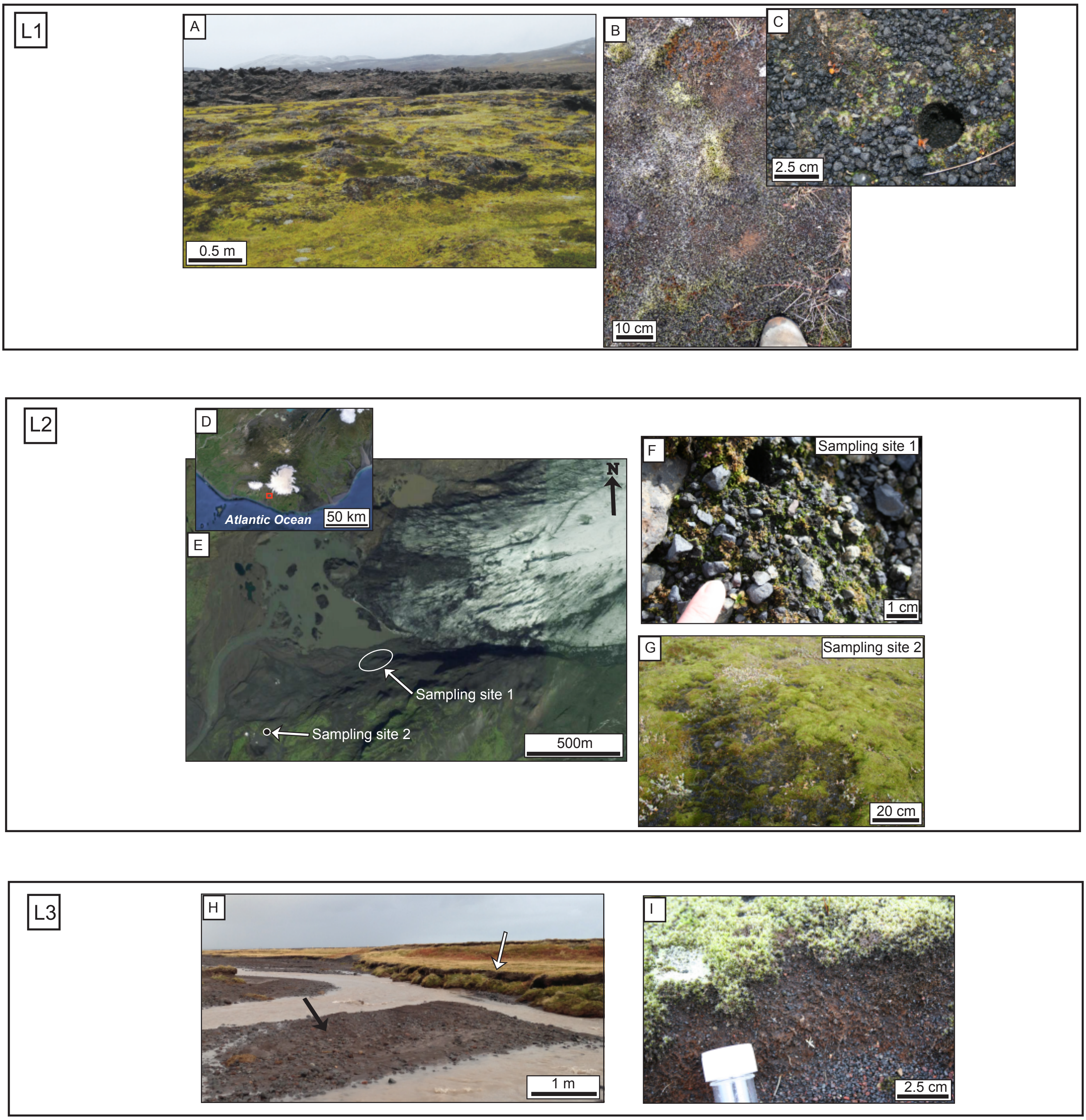

Table DR1 – Bryophyte species at each locality.

Locality no.	Location	Co-ordinates	Species present
L1	N. Krafla Fires	65 47.688'N 16 46.384'W	**Moss:** *Racomitrum spp., Ceratodon purpureus, Pohlia sp., Polytrichum juniperinum* **Liverwort:** *Scapania irrigua, Lophozia sudetica, Lophozia opacifolia, Aneura pinguis, Blasia pusilla.*
L2	Sólheimajökull glacier	63 31.960'N 19 21.458'W	**Moss:** *Racomitrium spp, Hypnum sp., Bryum sp, Pohlia bulbifera, Barbilophozia lycopodioides, Lophozia sudetica* **Liverwort:** *Blasia pusilla, Marchantia sp., Cephaloziella sp Jungermannia gracillima Scapania irrigua, Marchantia polymorpha subsp. montevagans, Nardia geoscyphus, Anthelia juratzkana, Lophozia wenzelii, Aneura pinguis.*
L3	Snæfellsnes Peninsula	64 52.149'N 23 50.673'W	**Moss:** *Racomitrium lanuginosum, Bartramia sp, Tetralophozia setiformis, Campylopus introflexus* **Liverwort:** *Barbilophozia barbata, Nardia geoscyphus, Lophozia sudetica, Lophozia obtuse, Lophozia bicrenata, Lophozia ventricosa, Nardia scalaris, Anthelia juratzkan., Barbilophozia kunzeana, Barbilophozia hatcheri, Diplophyllum albicans, Scapania cuspiduligera, Ptilidium ciliare.* **Other:** *Lycopodium fastigiatum.*

nb: This is not a comprehensive list of species present, and simply represents the species that were identified in the field and those that were collected for study on returning to the NHM.

Table DR2: Parameters for SEM and SEM-EDX data and image acquisition.

Image from main text	SEM	coated?	kv	spot size	WD	Detector	Pressure	Mode	Site
Fig. 2G	Quanta	n	10	3	11.5mm	LFD	70Pa	SE	L2 - Sólheimajökull (site 1)
Fig. 3A	Quanta	n	10	3	12mm	LFD	70Pa	SE	L2 - Sólheimajökull (site 1)
Fig. 3E	Quanta	y	10	3	14.5mm	ETD	1.41e-3Pa	SE	L3 - Snæfellsnes
Fig. 3F	Quanta	y	10	3	14.5mm	ETD	1.01e-3Pa	SE	L3 - Snæfellsnes
Fig. 2F	Leo	n	20	530	16mm	BSD	21Pa	VP	L2 - Sólheimajökull (site 2)
Fig. 3B	Leo	n	20	550	13mm	BSD	20Pa	VP	L1 - Krafla Fires
Fig. 3C	Leo	n	20	550	15mm	BSD	20Pa	VP	L3 - Snæfellsnes
Fig. 3D	Leo	n	20	530	16mm	BSD	21Pa	VP	L1 - Krafla Fires

Table DR3: Geochemical data in oxide weight %; average from 30 measurements at each site. Standard deviation shown in italics. Composition determined by SEM-EDX analysis on the Quanta SEM.

	SiO2	**FeO**	**Al2O3**	**CaO**	**TiO2**	**Mg0**	**Na2O**	**K2O**	**P205**	**TOTAL**
Bio-med	52.10	25.03	8.46	7.78	2.20	1.85	1.26	0.88	0.44	99.99
Fresh/clean	52.82	14.64	8.87	13.04	2.68	3.48	2.19	2.15	0.13	100.00
Bio-med st dev	*5.22*	*6.72*	*1.01*	*1.95*	*1.35*	*0.75*	*0.48*	*0.57*	*0.37*	
Fresh/clean st dev	*5.73*	*7.51*	*2.88*	*6.03*	*1.40*	*1.64*	*0.96*	*2.37*	*0.14*	

Table DR4: Grain and mineral types found in soils from each locality (L1-L3). Glass shards and scoria make up over 70% in each sample.

	Lithic		**Glass**		**Mineral**				
Site	Mafic	Felsic	Shard	Scoria	Quartz	Feldspar	Olivine	Pyroxene	Mica
L1	X		X	X	X	X			
L2	X	X	X	X	X			X	
L3	X	X	X	X	X	X		X	